O'REILLY®

3rd Edition

Hands-on Machine Learning with Scikit-Learn, Keras & TensorFlow

Concepts, Tools, and Techniques to Build Intelligent Systems

Early Release

RAW & UNEDITED

Aurélien Géron

Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow

THIRD EDITION

Concepts, Tools, and Techniques to Build Intelligent Systems

Aurélien Géron

Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow

by Aurélien Géron

Printed in the United States of America.

Published by O'Reilly Media, Inc., 1005 Gravenstein Highway North, Sebastopol, CA 95472.

O'Reilly books may be purchased for educational, business, or sales promotional use. Online editions are also available for most titles (http://oreilly.com). For more information, contact our corporate/institutional sales department: 800-998-9938 or *corporate@oreilly.com*.

Acquisitions Editor: Rebecca Novack

Development Editor: Nicole Taché

Production Editor: Beth Kelly

Copyeditor:

Proofreader:

Indexer:

Interior Designer: David Futato

Cover Designer: Karen Montgomery

Illustrator: Kate Dullea

October 2022: Third Edition

Revision History for the Early Release

- 2022-02-08: First Release
- 2022-03-14: Second Release

See http://oreilly.com/catalog/errata.csp?isbn=9781492032649 for release details.

978-1-098-12244-7

[]

Preface

The Machine Learning Tsunami

In 2006, Geoffrey Hinton et al. published a paper[1] showing how to train a deep neural network capable of recognizing handwritten digits with state-of-the-art precision (>98%). They branded this technique "Deep Learning." A deep neural network is a (very) simplified model of our cerebral cortex, composed of a stack of layers of artificial neurons. Training a deep neural net was widely considered impossible at the time,[2] and most researchers had abandoned the idea in the late 1990s. This paper revived the interest of the scientific community, and before long many new papers demonstrated that Deep Learning was not only possible, but capable of mind-blowing achievements that no other Machine Learning (ML) technique could hope to match (with the help of tremendous computing power and great amounts of data). This enthusiasm soon extended to many other areas of Machine Learning.

A decade later, Machine Learning had conquered the industry, and today it is at the heart of much of the magic in high-tech products, ranking your web search results, powering your smartphone's speech recognition, recommending videos, and beating the world champion at the game of Go. Before you know it, it will be driving your car.

Machine Learning in Your Projects

So, naturally you are excited about Machine Learning and would love to join the party!

Perhaps you would like to give your homemade robot a brain of its own? Make it recognize faces? Or learn to walk around?

Or maybe your company has tons of data (user logs, financial data, production data, machine sensor data, hotline stats, HR reports, etc.), and more than likely you could unearth some hidden gems if you just knew where to look. With Machine Learning, you could accomplish the following and much more:

- Segment customers and find the best marketing strategy for each group.
- Recommend products for each client based on what similar clients bought.
- Detect which transactions are likely to be fraudulent.
- Forecast next year's revenue.

Whatever the reason, you have decided to learn Machine Learning and implement it in your projects. Great idea!

Objective and Approach

This book assumes that you know close to nothing about Machine Learning. Its goal is to give you the concepts, tools, and intuition you need to implement programs capable of *learning from data*.

We will cover a large number of techniques, from the simplest and most commonly used (such as Linear Regression) to some of the Deep Learning techniques that regularly win competitions.

Rather than implementing our own toy versions of each algorithm, we will be using production-ready Python frameworks:

- Scikit-Learn is very easy to use, yet it implements many Machine Learning algorithms efficiently, so it makes for a great entry point to learning Machine Learning. It was created by David Cournapeau in 2007, and is now led by a team of researchers at the French Institute for Research in Computer Science and Automation (Inria).

- TensorFlow is a more complex library for distributed numerical computation. It makes it possible to train and run very large neural networks efficiently by distributing the computations across potentially hundreds of multi-GPU (graphics processing unit) servers. TensorFlow (TF) was created at Google and supports many of its large-scale Machine Learning applications. It was open sourced in November 2015, and version 2.0 was released in September 2019.
- Keras is a high-level Deep Learning API that makes it very simple to train and run neural networks. Keras comes bundled with TensorFlow, and it relies on TensorFlow for all the intensive computations.

The book favors a hands-on approach, growing an intuitive understanding of Machine Learning through concrete working examples and just a little bit of theory.

> **TIP**
>
> While you can read this book without picking up your laptop, I highly recommend you experiment with the code examples available online. See the *Code examples* section later in this preface.

Prerequisites

This book assumes that you have some Python programming experience. If you don't know Python yet, *https://learnpython.org/* is a great place to start. The official tutorial on Python.org is also quite good.

This book also assumes that you are familiar with Python's main scientific libraries—in particular, NumPy, Pandas, and Matplotlib. If you have never used these libraries, don't worry, they're easy to learn, and I created a tutorial for each of them. You can access them online at *https://homl.info/tutorials*.

Moreover, if you want to fully understand how the Machine Learning algorithms work (not just how to use them), then you should have at least a basic understanding of a few math concepts, especially linear algebra. Specifically, you should know what vectors and matrices are, and how to perform some simple operations like adding vectors, or transposing and multiplying matrices. If you need a quick introduction to linear algebra (it's really not rocket science!), I created a tutorial available at *https://homl.info/tutorials*. You will also find a tutorial on differential calculus, which may be helpful to understand how neural networks are trained, but it's not entirely essential to grasp the important concepts. This book also uses other mathematical concepts occasionally, such as exponentials and logarithms, a bit of probability theory and some basic statistics concepts, but nothing too advanced. If you need help on any of these, please check out *https://khanacademy.org/*, which offers many excellent and free math courses online.

Roadmap

This book is organized in two parts. Part I, "The Fundamentals of Machine Learning", covers the following topics:

- What Machine Learning is, what problems it tries to solve, and the main categories and fundamental concepts of its systems
- The steps in a typical Machine Learning project
- Learning by fitting a model to data
- Optimizing a cost function
- Handling, cleaning, and preparing data
- Selecting and engineering features
- Selecting a model and tuning hyperparameters using cross-validation

- The challenges of Machine Learning, in particular underfitting and overfitting (the bias/variance trade-off)
- The most common learning algorithms: Linear and Polynomial Regression, Logistic Regression, k-Nearest Neighbors, Support Vector Machines, Decision Trees, Random Forests, and Ensemble methods
- Reducing the dimensionality of the training data to fight the "curse of dimensionality"
- Other unsupervised learning techniques, including clustering, density estimation, and anomaly detection

Part II, "Neural Networks and Deep Learning", covers the following topics:

- What neural nets are and what they're good for
- Building and training neural nets using TensorFlow and Keras
- The most important neural net architectures: feedforward neural nets for tabular data, convolutional nets for computer vision, recurrent nets and long short-term memory (LSTM) nets for sequence processing, encoder/decoders and Transformers for natural language processing, autoencoders and generative adversarial networks (GANs) for generative learning
- Techniques for training deep neural nets
- How to build an agent (e.g., a bot in a game) that can learn good strategies through trial and error, using Reinforcement Learning
- Loading and preprocessing large amounts of data efficiently
- Training and deploying TensorFlow models at scale

The first part is based mostly on Scikit-Learn, while the second part uses TensorFlow and Keras.

CAUTION

Don't jump into deep waters too hastily: while Deep Learning is no doubt one of the most exciting areas in Machine Learning, you should master the fundamentals first. Moreover, most problems can be solved quite well using simpler techniques such as Random Forests and Ensemble methods (discussed in Part I). Deep Learning is best suited for complex problems such as image recognition, speech recognition, or natural language processing, and it requires a lot of data, computing power, and patience (unless you can leverage a pre-trained neural network, as we will see).

Changes in the Third Edition

This third edition has four main objectives:

1. Cover additional ML topics: (TODO write the list of new ML topics)
2. Discuss some of the latest important results from Deep Learning research.
3. Update the code examples to use the latest versions of Scikit-Learn, NumPy, Pandas, Matplotlib, and other libraries.
4. Clarify some sections and fix some errors, thanks to plenty of great feedback from readers.

See *https://homl.info/changes3* for more details on what changed in the third edition. (TODO write changes page and link to it)

Code Examples

All the code examples in this book are open source and available online at *https://github.com/ageron/handson-ml3*, as Jupyter notebooks. These are interactive documents containing text, images, and executable code snippets (Python in our case). The easiest and quickest way to get started is to run these notebooks using Google Colab: this is a free service that allows you to run any Jupyter notebook directly online, without having to install anything on your machine. All you need is a web browser and a Google account.

> **NOTE**
>
> In this book, I will assume that you are using Google Colab, but I have also tested the notebooks on other online platforms such as Kaggle or Binder, so you can use those if you prefer. Alternatively, you can install the required libraries and tools (or the Docker image for this book) and run the notebooks directly on your own machine. See the instructions at *https://github.com/ageron/handson-ml3*.

Other Resources

Many excellent resources are available to learn about Machine Learning. For example, Andrew Ng's ML course on Coursera is amazing, although it requires a significant time investment.

There are also many interesting websites about Machine Learning, including of course Scikit-Learn's exceptional User Guide. You may also enjoy Dataquest, which provides very nice interactive tutorials, and ML blogs such as those listed on Quora. Finally, there are many excellent YouTube channels about Machine Learning, including ML Street Talk, Yannic Kilcher and many others, some of which are listed at *https://homl.info/youtubechannels*.

There are many other introductory books about Machine Learning. In particular:

- Joel Grus's *Data Science from Scratch*, 2nd edition (O'Reilly) presents the fundamentals of Machine Learning and implements some of the main algorithms in pure Python (from scratch, as the name suggests).

- Stephen Marsland's *Machine Learning: An Algorithmic Perspective*, 2nd edition (Chapman & Hall) is a great introduction to Machine Learning, covering a wide range of topics in depth with code examples in Python (also from scratch, but using NumPy).

- Sebastian Raschka's *Python Machine Learning*, 3rd edition (Packt Publishing) is also a great introduction to Machine Learning and leverages Python open source libraries (Pylearn 2 and Theano).
- François Chollet's *Deep Learning with Python*, 2nd edition (Manning) is a very practical book that covers a large range of topics in a clear and concise way, as you might expect from the author of the excellent Keras library. It favors code examples over mathematical theory.
- Andriy Burkov's *The Hundred-Page Machine Learning Book* is very short and covers an impressive range of topics, introducing them in approachable terms without shying away from the math equations.
- Yaser S. Abu-Mostafa, Malik Magdon-Ismail, and Hsuan-Tien Lin's *Learning from Data* (AMLBook) is a rather theoretical approach to ML that provides deep insights, in particular on the bias/variance trade-off (see Chapter 4).
- Stuart Russell and Peter Norvig's *Artificial Intelligence: A Modern Approach*, 4th Edition (Pearson), is a great (and huge) book covering an incredible amount of topics, including Machine Learning. It helps put ML into perspective.
- Jeremy Howard and Sylvain Gugger's *Deep Learning for Coders with fastai and PyTorch* (O'Reilly) provides a wonderfully clear and practical introduction to Deep Learning using the fastai and PyTorch libraries.

Finally, joining ML competition websites such as Kaggle.com will allow you to practice your skills on real-world problems, with help and insights from some of the best ML professionals out there.

Conventions Used in This Book

The following typographical conventions are used in this book:

Italic

Indicates new terms, URLs, email addresses, filenames, and file extensions.

`Constant width`

Used for program listings, as well as within paragraphs to refer to program elements such as variable or function names, databases, data types, environment variables, statements and keywords.

`Constant width bold`

Shows commands or other text that should be typed literally by the user.

`Constant width italic`

Shows text that should be replaced with user-supplied values or by values determined by context.

> **TIP**
>
> This element signifies a tip or suggestion.

> **NOTE**
>
> This element signifies a general note.

> **WARNING**
>
> This element indicates a warning or caution.

O’Reilly Online Learning

> **NOTE**
>
> For almost 40 years, *O’Reilly Media* has provided technology and business training, knowledge, and insight to help companies succeed.

Our unique network of experts and innovators share their knowledge and expertise through books, articles, and our online learning platform. O’Reilly’s online learning platform gives you on-demand access to live training courses, in-depth learning paths, interactive coding environments, and a vast collection of text and video from O’Reilly and 200+ other publishers. For more information, please visit *https://oreilly.com*.

How to Contact Us

Please address comments and questions concerning this book to the publisher:

O’Reilly Media, Inc.

1005 Gravenstein Highway North

Sebastopol, CA 95472

800-998-9938 (in the United States or Canada)

707-829-0515 (international or local)

707-829-0104 (fax)

We have a web page for this book, where we list errata, examples, and any additional information. You can access this page at *https://homl.info/oreilly2*.

To comment or ask technical questions about this book, send email to *bookquestions@oreilly.com*.

For news and more information about our books and courses, see our website at *https://www.oreilly.com*.

Find us on Facebook: *https://facebook.com/oreilly*

Follow us on Twitter: *https://twitter.com/oreillymedia*

Watch us on YouTube: *https://www.youtube.com/oreillymedia*

Acknowledgments

Never in my wildest dreams did I imagine that the first and second editions of this book would get such a large audience. I received so many messages from readers, many asking questions, some kindly pointing out errata, and most sending me encouraging words. I cannot express how grateful I am to all these readers for their tremendous support. Thank you all so very much! Please do not hesitate to file issues on GitHub if you find errors in the code examples (or just to ask questions), or to submit errata (TODO define link) if you find errors in the text. Some readers also shared how this book helped them get their first job, or how it helped them solve a concrete problem they were working on. I find such feedback incredibly motivating. If you find this book helpful, I would love it if you could share your story with me, either privately (e.g., via LinkedIn) or publicly (e.g., tweet me at @aureliengeron or write an Amazon review). (TODO define link)

(TODO: add thanks to 3rd edition reviewers: Hannes Hapke, Sara Robinson, Laurence Moroney, Kyle Gallatin, Eric Lebigot, Jason Mayes, Soonson Kwon and Google for GCE credits)

(TODO: add thanks to Ulf Bissbort for ML discussions)

(TODO update this paragraph for 3rd edition) Many thanks as well to O’Reilly’s fantastic staff, in particular Nicole Taché, who gave me insightful feedback and was always cheerful, encouraging, and helpful: I could not dream of a better editor. Big thanks to Michele Cronin as well, who was very helpful (and patient) at the start of this second edition, and to Kristen Brown, the production editor for the second edition, who saw it through all the steps (she also coordinated fixes and updates for each reprint of the first edition). Thanks as well to Rachel Monaghan and Amanda Kersey for their thorough copyediting (respectively for the first and second edition), and to Johnny O'Toole who managed the relationship with Amazon and answered many of my questions. Thanks to Marie Beaugureau, Ben Lorica, Mike Loukides, and Laurel Ruma for believing in this project and helping me define its scope. Thanks to Matt Hacker and all of the Atlas team for answering all my technical questions regarding formatting, AsciiDoc, and LaTeX, and thanks to Nick Adams, Rebecca Demarest, Rachel Head, Judith McConville, Helen Monroe, Karen Montgomery, Rachel Roumeliotis, and everyone else at O'Reilly who contributed to this book.

I'll never forget all the wonderful people who helped me with the first and second editions of this book: friends, colleagues, experts, including many members of the TensorFlow team, the list is long: Olzhas Akpambetov, Karmel Allison, Martin Andrews, David Andrzejewski, Paige Bailey, Lukas Biewald, Eugene Brevdo, William Chargin, François Chollet, Robert Crowe, Mark Daoust, Daniel "Wolff" Dobson, Nick Felt, Bruce Fontaine, Justin Francis, Goldie Gadde, Irene Giannoumis, Ingrid von Glehn, Vincent Guilbeau, Sandeep Gupta, Priya Gupta, Kevin Haas, Eddy Hung, Konstantinos Katsiapis, Viacheslav Kovalevskyi, Jon Krohn, Allen Lavoie, Karim Matrah, Grégoire Mesnil, Clemens Mewald, Dan Moldovan, Dominic Monn, Sean Morgan, Tom O'Malley, Haesun Park, Alexandre Passos, Ankur Patel, Josh Patterson, André Susano Pinto, Anthony Platanios, Oscar Ramirez, Anna Revinskaya, Saurabh Saxena, Salim Sémaoune, Ryan Sepassi, Jiri Simsa, Iain Smears, Xiaodan Song, Christina Sorokin, Michel Tessier, Dustin Tran, Todd Wang, Pete Warden, Martin Wicke, Edd Wilder-James, Sam Witteveen, Jason Zaman, Yuefeng Zhou and my dear brother Sylvain.

I would also like to thank my former Google colleagues, in particular the YouTube video classification team, for teaching me so much about Machine

Learning. I could never have started the first edition without them. Special thanks to my personal ML gurus: Clément Courbet, Julien Dubois, Mathias Kende, Daniel Kitachewsky, James Pack, Alexander Pak, Anosh Raj, Vitor Sessak, Wiktor Tomczak, Ingrid von Glehn, and Rich Washington. And thanks to everyone else I worked with at YouTube and in the amazing Google research teams in Mountain View.

Last but not least, I am infinitely grateful to my beloved wife, Emmanuelle, and to our three wonderful children, Alexandre, Rémi, and Gabrielle, for encouraging me to work hard on this book. I'm also thankful to them for their insatiable curiosity: explaining some of the most difficult concepts in this book to my wife and children helped me clarify my thoughts and directly improved many parts of it. And they keep bringing me cookies and coffee, who could ask for anything more?

---

1 Geoffrey E. Hinton et al., "A Fast Learning Algorithm for Deep Belief Nets," *Neural Computation* 18 (2006): 1527–1554.

2 Despite the fact that Yann LeCun's deep convolutional neural networks had worked well for image recognition since the 1990s, although they were not as general-purpose.

Part I. The Fundamentals of Machine Learning

Chapter 1. The Machine Learning Landscape

> **A NOTE FOR EARLY RELEASE READERS**
>
> With Early Release ebooks, you get books in their earliest form—the author’s raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.
>
> This will be the 1st chapter of the final book. Notebooks are available on GitHub at *https://github.com/ageron/handson-ml3*. Datasets are available at *https://github.com/ageron/data*.
>
> If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the editoor at ntache@oreilly.com.

Not so long ago, if you had picked up your phone and asked it the way home, it would have ignored you—and people would have questionned your sanity. But Machine Learning is no longer Science Fiction: billions of people use it every day. And the truth is it has actually been around for decades in some specialized applications, such as Optical Character Recognition (OCR). The first ML application that really became mainstream, improving the lives of hundreds of millions of people, took over the world back in the 1990s: the *spam filter*. It’s not exactly a self-aware robot, but it does technically qualify as Machine Learning: it has actually learned so well that you seldom need to flag an email as spam anymore. It was followed by hundreds of ML applications that now quietly power hundreds of products and features that you use regularly: voice prompts, automatic translation, image search, product recommendations, and many more.

Where does Machine Learning start and where does it end? What exactly does it mean for a machine to *learn* something? If I download a copy of all Wikipedia articles, has my computer really learned something? Is it suddenly smarter? In this chapter I will start by clarifying what Machine Learning is and why you may want to use it.

Then, before we set out to explore the Machine Learning continent, we will take a look at the map and learn about the main regions and the most notable landmarks: supervised versus unsupervised learning and their variants, online versus batch learning, instance-based versus model-based learning. Then we will look at the workflow of a typical ML project, discuss the main challenges you may face, and cover how to evaluate and fine-tune a Machine Learning system.

This chapter introduces a lot of fundamental concepts (and jargon) that every data scientist should know by heart. It will be a high-level overview (it's the only chapter without much code), all rather simple, but my goal is to ensure everything is crystal clear to you before we continue on to the rest of the book. So grab a coffee and let's get started!

> **TIP**
>
> If you are already familiar with Machine Learning basics, you may want to skip directly to Chapter 2. If you are not sure, try to answer all the questions listed at the end of the chapter before moving on.

What Is Machine Learning?

Machine Learning is the science (and art) of programming computers so they can *learn from data*.

Here is a slightly more general definition:

> *[Machine Learning is the] field of study that gives computers the ability to learn without being explicitly programmed.*
>
> —Arthur Samuel，1959

And a more engineering-oriented one:

> *A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E.*
>
> —Tom Mitchell，1997

Your spam filter is a Machine Learning program that, given examples of spam emails (flagged by users) and examples of regular emails (nonspam, also called "ham"), can learn to flag spam. The examples that the system uses to learn are called the *training set*. Each training example is called a *training instance* (or *sample*). The part of a Machine Learning system that learns and makes predictions is called a *model*. Neural networks and random forests are examples of models.

In this case, the task *T* is to flag spam for new emails, the experience *E* is the *training data*, and the performance measure *P* needs to be defined; for example, you can use the ratio of correctly classified emails. This particular performance measure is called *accuracy*, and it is often used in classification tasks.

If you just download a copy of all Wikipedia articles, your computer has a lot more data, but it is not suddenly better at any task. It is not Machine Learning.

Why Use Machine Learning?

Consider how you would write a spam filter using traditional programming techniques (Figure 1-1):

1. First you would examine what spam typically looks like. You might notice that some words or phrases (such as "4U," "credit card," "free," and "amazing") tend to come up a lot in the subject line. Perhaps you would also notice a few other patterns in the sender's name, the email's body, and other parts of the email.

2. You would write a detection algorithm for each of the patterns that you noticed, and your program would flag emails as spam if a number of these patterns were detected.
3. You would test your program and repeat steps 1 and 2 until it was good enough to launch.

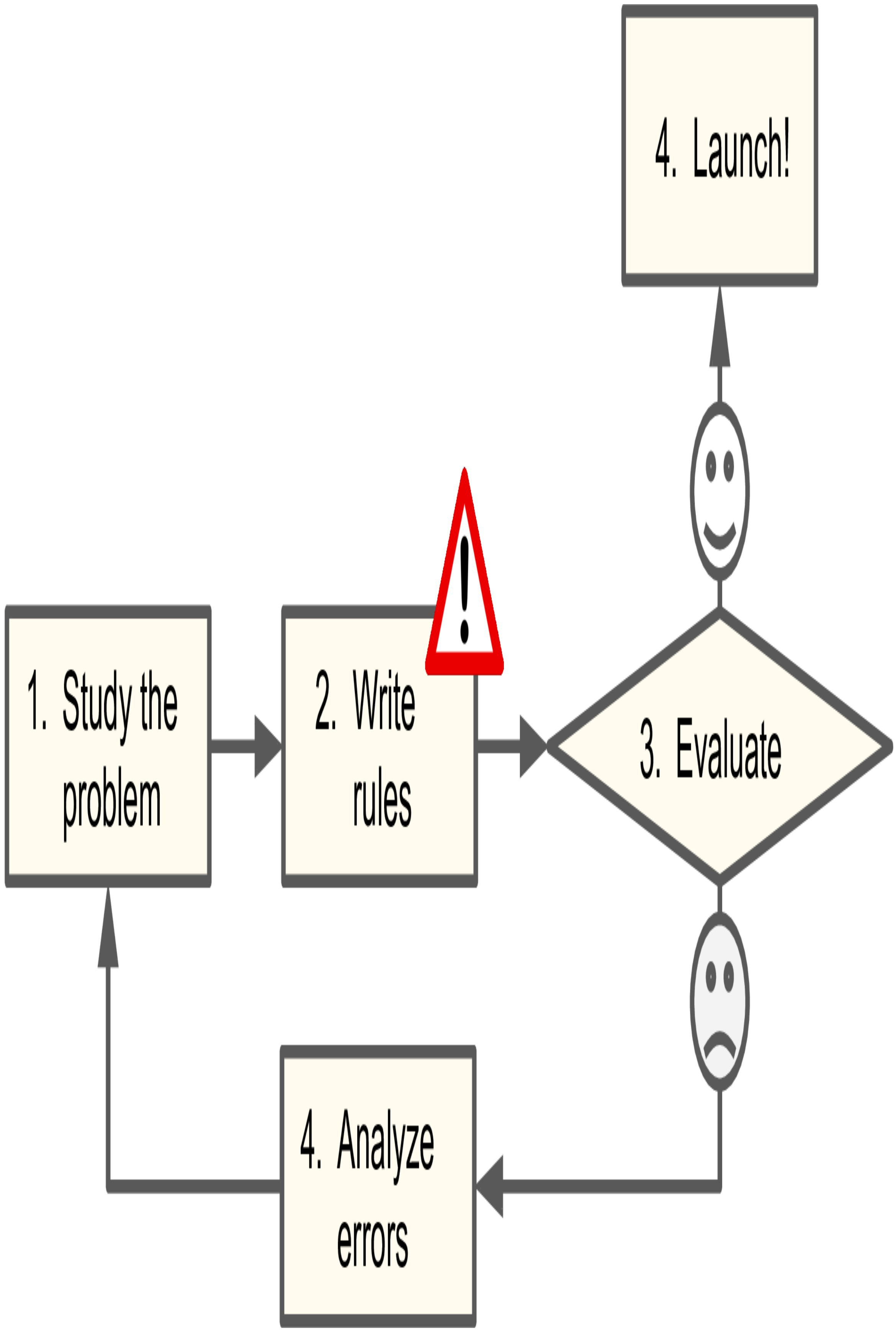

4. Launch!
1. Study the problem
2. Write rules
3. Evaluate
4. Analyze errors

Figure 1-1. The traditional approach

Since the problem is difficult, your program will likely become a long list of complex rules—pretty hard to maintain.

In contrast, a spam filter based on Machine Learning techniques automatically learns which words and phrases are good predictors of spam by detecting unusually frequent patterns of words in the spam examples compared to the ham examples (Figure 1-2). The program is much shorter, easier to maintain, and most likely more accurate.

What if spammers notice that all their emails containing “4U” are blocked? They might start writing “For U” instead. A spam filter using traditional programming techniques would need to be updated to flag “For U” emails. If spammers keep working around your spam filter, you will need to keep writing new rules forever.

In contrast, a spam filter based on Machine Learning techniques automatically notices that “For U” has become unusually frequent in spam flagged by users, and it starts flagging them without your intervention (Figure 1-3).

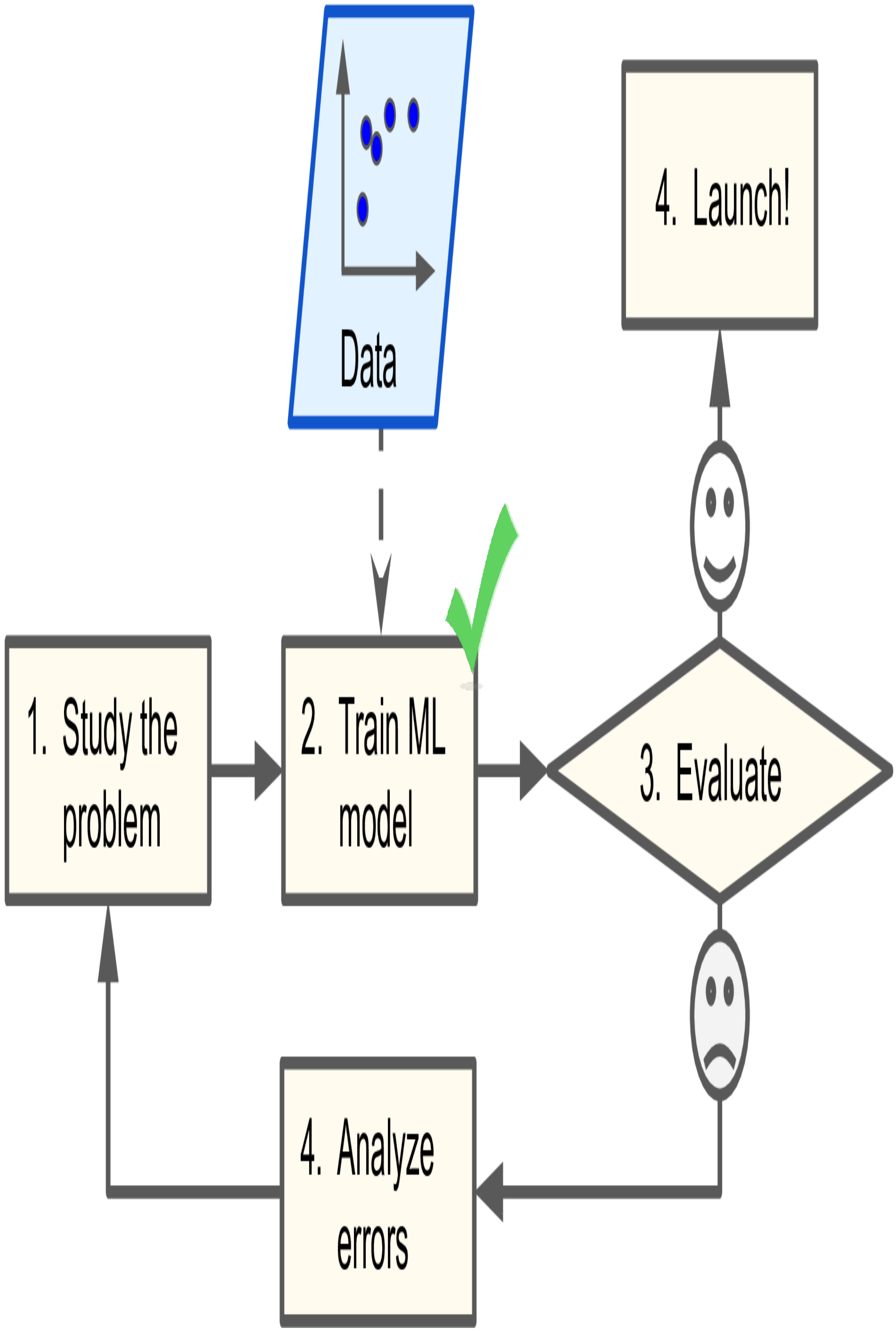

Data
4. Launch!
1. Study the problem
2. Train ML model
3. Evaluate
4. Analyze errors

Figure 1-2. The Machine Learning approach

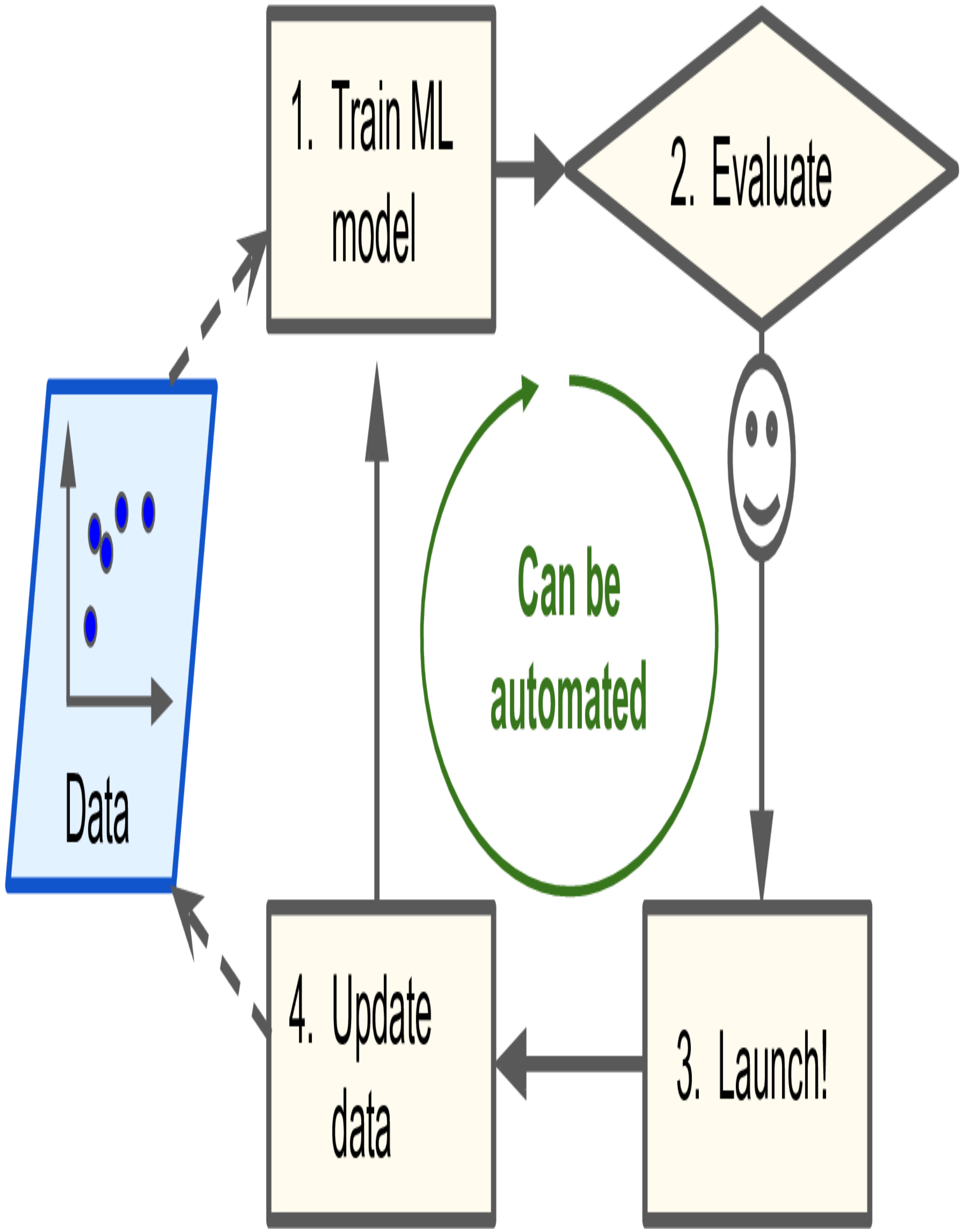


Figure 1-3. Automatically adapting to change

Another area where Machine Learning shines is for problems that either are too complex for traditional approaches or have no known algorithm. For example, consider speech recognition. Say you want to start simple and write a program capable of distinguishing the words "one" and "two." You might notice that the word "two" starts with a high-pitch sound ("T"), so you could hardcode an algorithm that measures high-pitch sound intensity and use that to distinguish ones and twos—but obviously this technique will not scale to thousands of words spoken by millions of very different people in noisy environments and in dozens of languages. The best solution (at least today) is to write an algorithm that learns by itself, given many example recordings for each word.

Finally, Machine Learning can help humans learn (Figure 1-4). ML models can be inspected to see what they have learned (although for some models this can be tricky). For instance, once a spam filter has been trained on enough spam, it can easily be inspected to reveal the list of words and combinations of words that it believes are the best predictors of spam. Sometimes this will reveal unsuspected correlations or new trends, and thereby lead to a better understanding of the problem. Digging into large amounts of data to discover hidden patterns is called *data mining*, and Machine Learning excels at it.

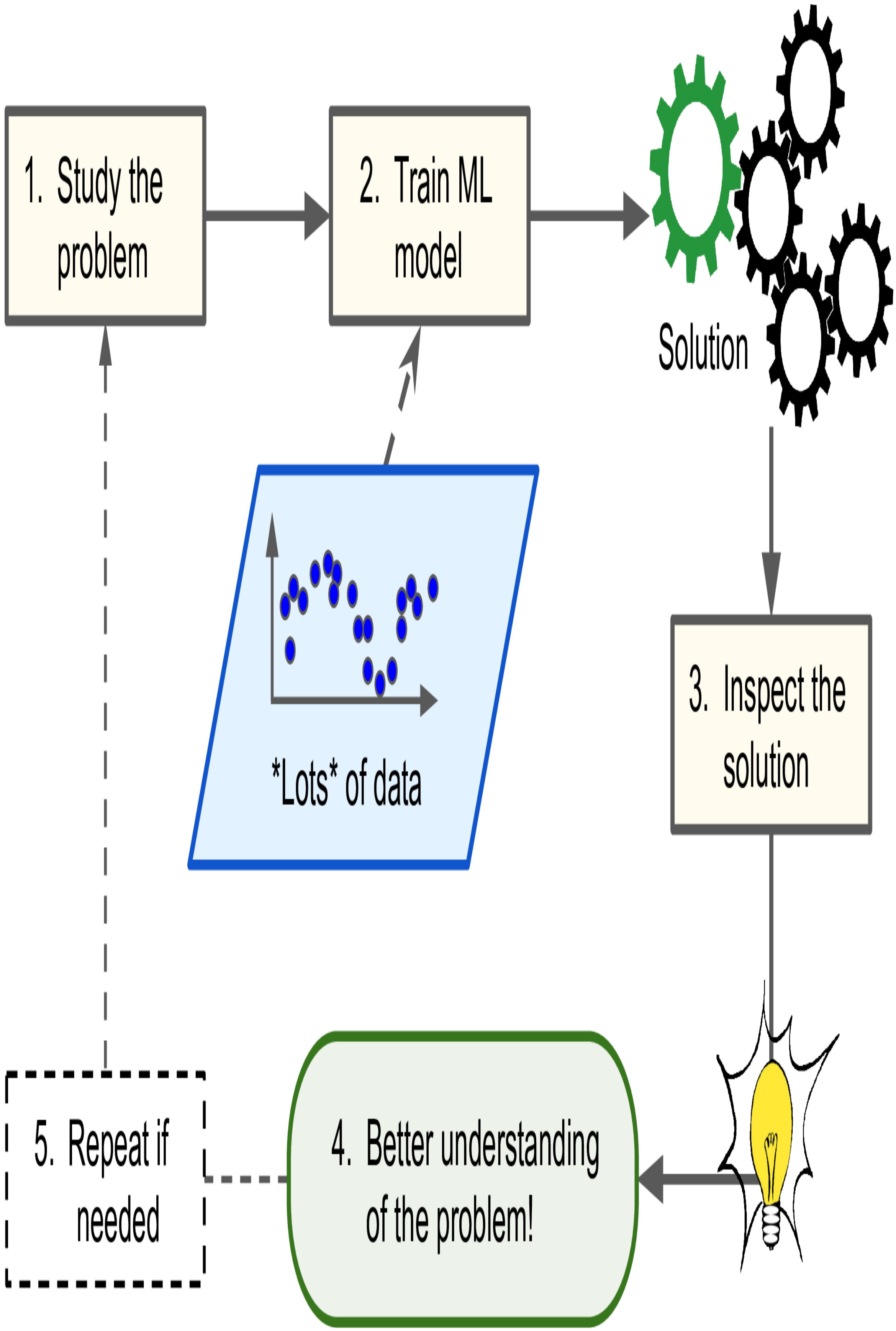

1. Study the problem
2. Train ML model
Solution
Lots of data
3. Inspect the solution
4. Better understanding of the problem!
5. Repeat if needed

Figure 1-4. Machine Learning can help humans learn

To summarize, Machine Learning is great for:

- Problems for which existing solutions require a lot of fine-tuning or long lists of rules: one Machine Learning model can often simplify code and perform better than the traditional approach.
- Complex problems for which using a traditional approach yields no good solution: the best Machine Learning techniques can perhaps find a solution.
- Fluctuating environments: a Machine Learning system can easily be retrained on new data, always keeping it up to date.
- Getting insights about complex problems and large amounts of data.

Examples of Applications

Let's look at some concrete examples of Machine Learning tasks, along with the techniques that can tackle them:

Analyzing images of products on a production line to automatically classify them

This is image classification, typically performed using convolutional neural networks (CNNs; see Chapter 14) or sometimes Transformers (see Chapter 16).

Detecting tumors in brain scans

This is semantic image segmentation, where each pixel in the image is classified (as we want to determine the exact location and shape of tumors), typically using CNNs or Transformers.

Automatically classifying news articles

This is natural language processing (NLP), and more specifically text classification, which can be tackled using recurrent neural networks (RNNs) and CNNs, but Transformers work even better (see Chapter 16).

Automatically flagging offensive comments on discussion forums

This is also text classification, using the same NLP tools.

Summarizing long documents automatically

This is a branch of NLP called text summarization, again using the same tools.

Creating a chatbot or a personal assistant

This involves many NLP components, including natural language understanding (NLU) and question-answering modules.

Forecasting your company's revenue next year, based on many performance metrics

This is a regression task (i.e., predicting values) that may be tackled using any regression model, such as a Linear Regression or Polynomial Regression model (see Chapter 4), a regression SVM (see Chapter 5), a regression Random Forest (see Chapter 7), or an artificial neural network (see Chapter 10). If you want to take into account sequences of past performance metrics, you may want to use RNNs, CNNs, or Transformers (see Chapters 15 and 16).

Making your app react to voice commands

This is speech recognition, which requires processing audio samples: since they are long and complex sequences, they are typically processed using RNNs, CNNs, or Transformers (see Chapters 15 and 16).

Detecting credit card fraud

This is anomaly detection, which can be tackled using isolation forests, Gaussian mixture models (see Chapter 9) or autoencoders (see Chapter 17).

Segmenting clients based on their purchases so that you can design a different marketing strategy for each segment

This is clustering, which can be achieved using K-Means, DBSCAN and more (see Chapter 9).

Representing a complex, high-dimensional dataset in a clear and insightful diagram

This is data visualization, often involving dimensionality reduction techniques (see Chapter 8).

Recommending a product that a client may be interested in, based on past purchases

This is a recommender system. One approach is to feed past purchases (and other information about the client) to an artificial neural network (see Chapter 10), and get it to output the most likely next purchase. This neural net would typically be trained on past sequences of purchases across all clients.

Building an intelligent bot for a game

This is often tackled using Reinforcement Learning (RL; see Chapter 18), which is a branch of Machine Learning that trains agents (such as bots) to pick the actions that will maximize their rewards over time (e.g., a bot may get a reward every time the player loses some life points), within a given environment (such as the game). The famous AlphaGo program that beat the world champion at the game of Go was built using RL.

This list could go on and on, but hopefully it gives you a sense of the incredible breadth and complexity of the tasks that Machine Learning can tackle, and the types of techniques that you would use for each task.

Types of Machine Learning Systems

There are so many different types of Machine Learning systems that it is useful to classify them in broad categories, based on the following criteria:

- How they are supervised during training (supervised, unsupervised, semi-supervised, self-supervised, and others)
- Whether or not they can learn incrementally on the fly (online versus batch learning)
- Whether they work by simply comparing new data points to known data points, or instead by detecting patterns in the training data and building a predictive model, much like scientists do (instance-based versus model-based learning)

These criteria are not exclusive; you can combine them in any way you like. For example, a state-of-the-art spam filter may learn on the fly using a deep neural network model trained using human-provided examples of spam and ham; this makes it an online, model-based, supervised learning system.

Let's look at each of these criteria a bit more closely.

Training Supervision

ML systems can be classified according to the amount and type of supervision they get during training. There are many categories, but we'll discuss the main ones: supervised learning, unsupervised learning, self-supervised learning, semi-supervised learning, and Reinforcement Learning.

Supervised learning

In *supervised learning*, the training set you feed to the algorithm includes the desired solutions, called *labels* (Figure 1-5).

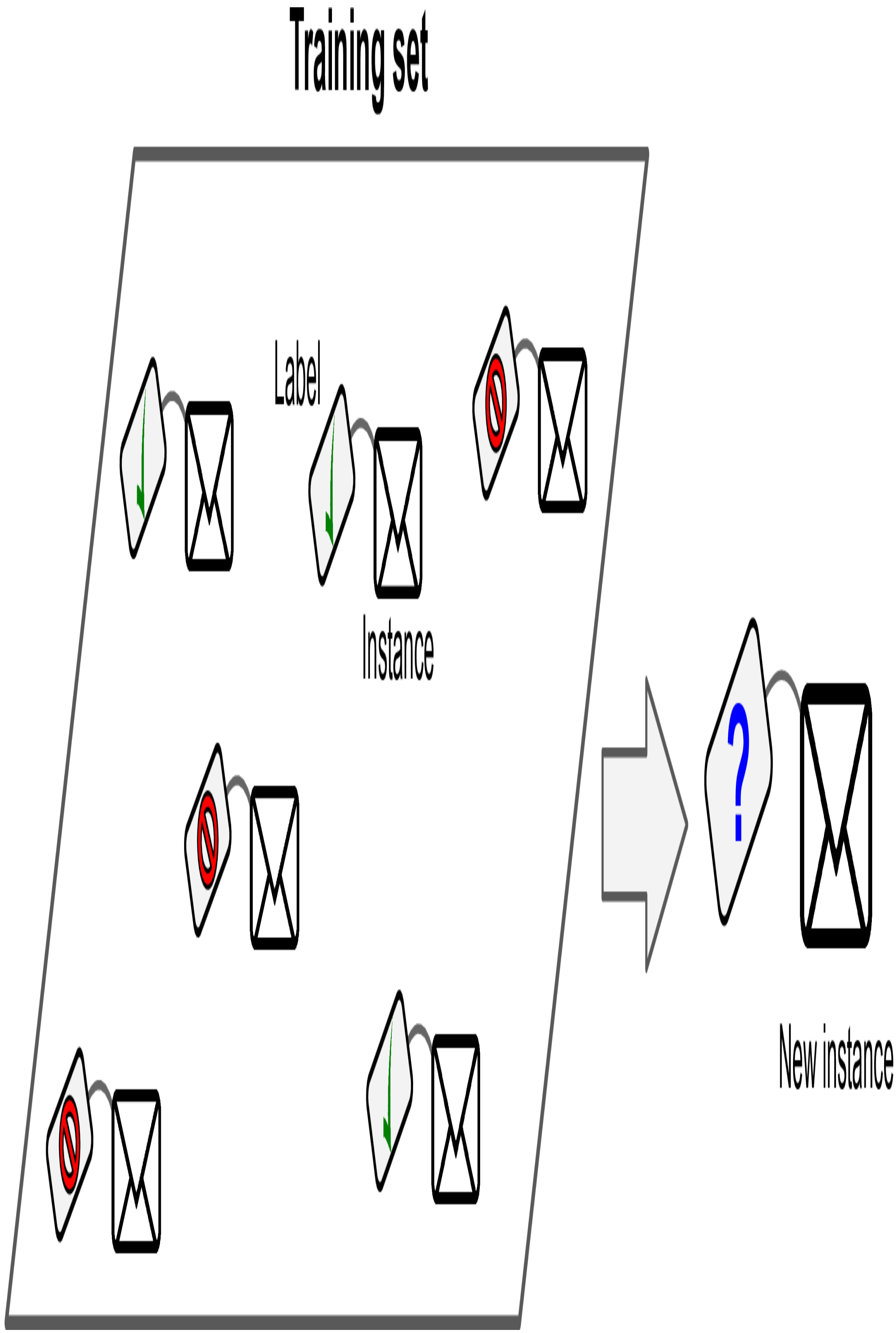

Training set
Label
Instance
New instance

Figure 1-5. A labeled training set for spam classification (an example of supervised learning)

A typical supervised learning task is *classification*. The spam filter is a good example of this: it is trained with many example emails along with their *class* (spam or ham), and it must learn how to classify new emails.

Another typical task is to predict a *target* numeric value, such as the price of a car, given a set of *features* (mileage, age, brand, etc.). This sort of task is called *regression* (Figure 1-6).[1] To train the system, you need to give it many examples of cars, including both their features and their targets (i.e., their prices).

> **NOTE**
>
> The words *target* and *label* are generally treated as synonyms in supervised learning, but *target* is more common in regression tasks, and *label* is more common in classification tasks. Moreover, *features* are sometimes called *predictors* or *attributes*. These terms may refer to individual samples (e.g., "this car's mileage feature is equal to 15,000") or to all samples (e.g., "the mileage feature is strongly correlated with price").

Note that some regression models can be used for classification as well, and vice versa. For example, *Logistic Regression* is commonly used for classification, as it can output a value that corresponds to the probability of belonging to a given class (e.g., 20% chance of being spam).

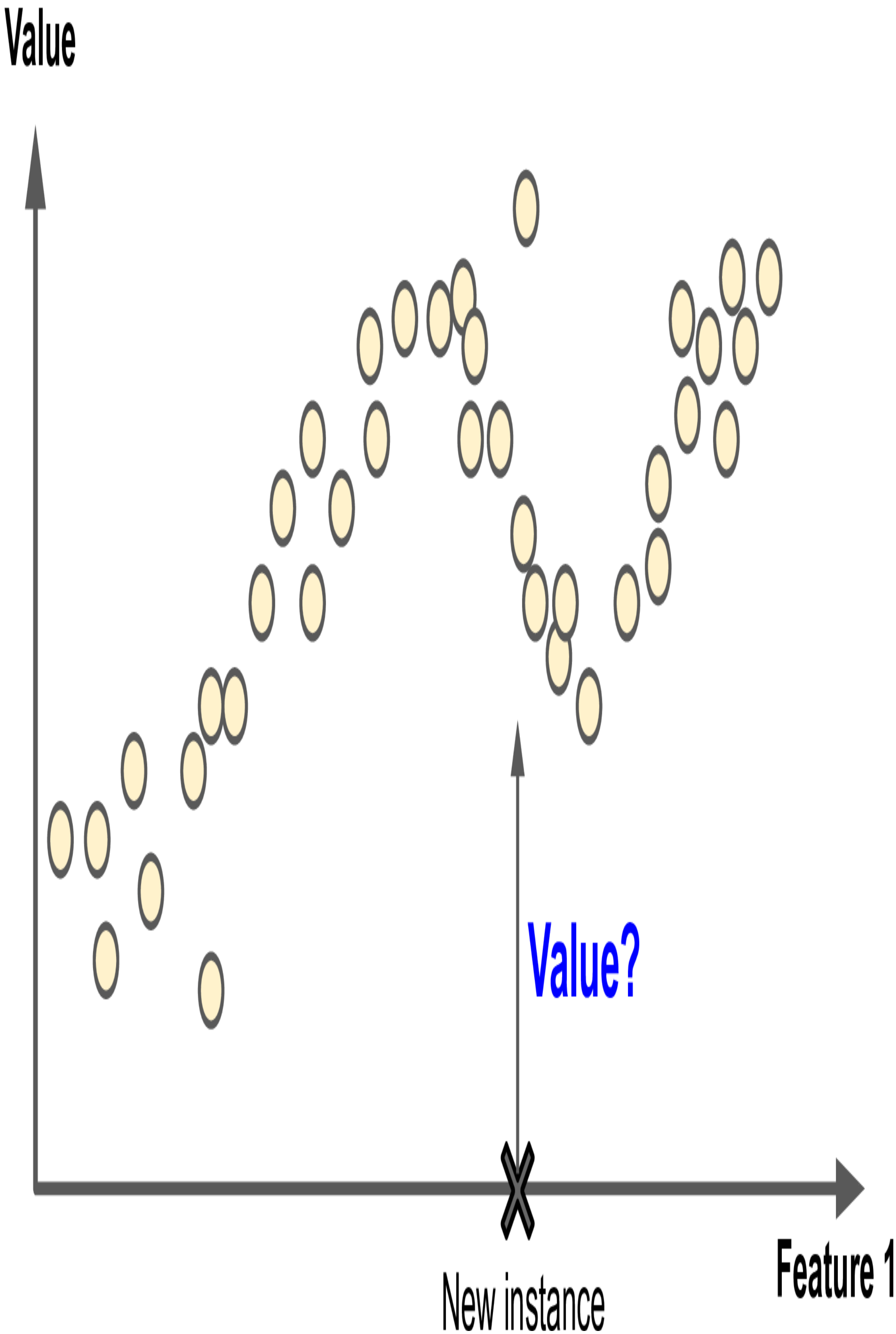

Value
Value?
New instance
Feature 1

Figure 1-6. A regression problem: predict a value, given an input feature (there are usually multiple input features, and sometimes multiple output values)

Unsupervised learning

In *unsupervised learning*, as you might guess, the training data is unlabeled (Figure 1-7). The system tries to learn without a teacher.

Training set

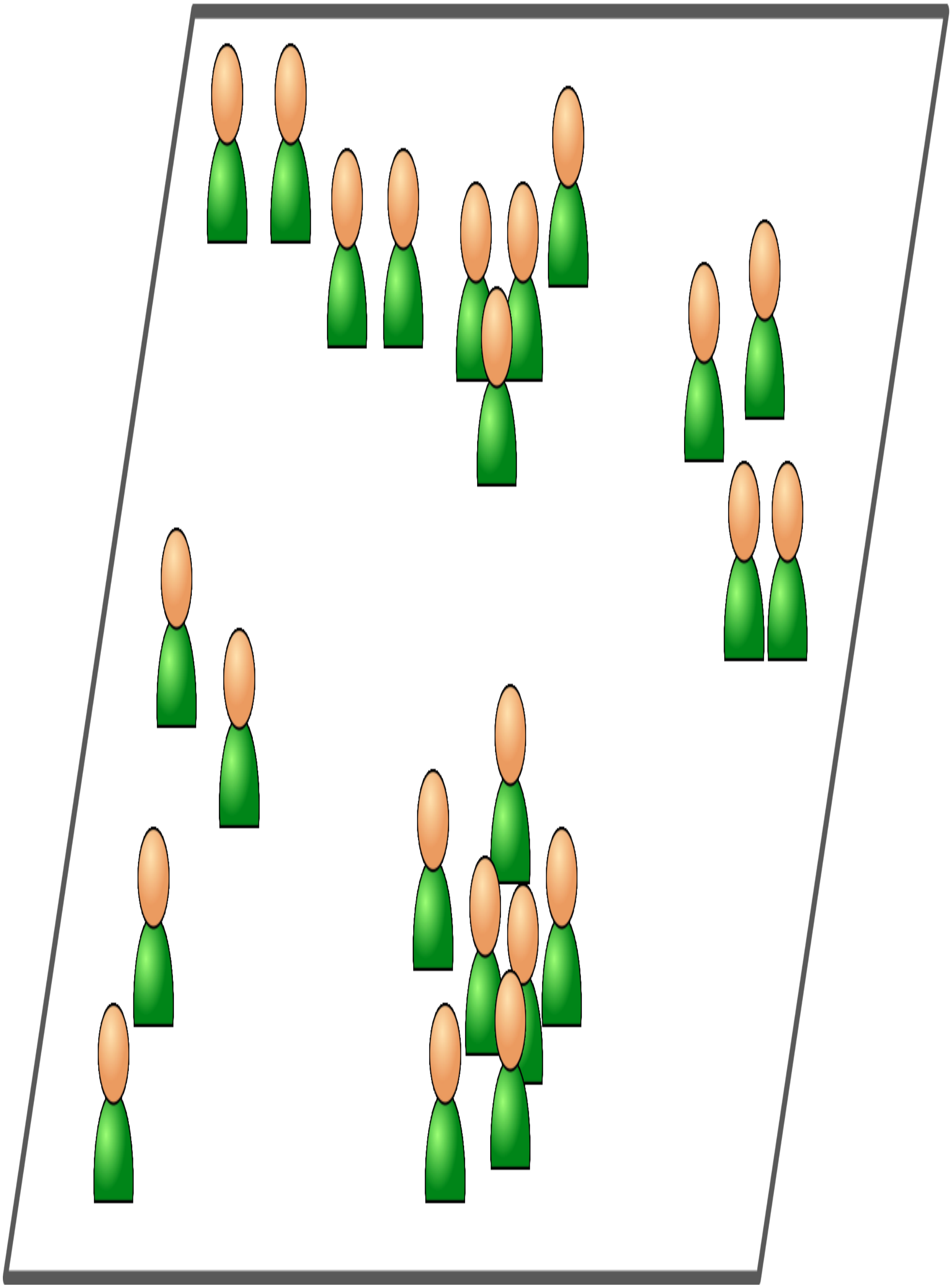


Figure 1-7. An unlabeled training set for unsupervised learning

For example, say you have a lot of data about your blog's visitors. You may want to run a *clustering* algorithm to try to detect groups of similar visitors (Figure 1-8). At no point do you tell the algorithm which group a visitor belongs to: it finds those connections without your help. For example, it might notice that 40% of your visitors are teenagers who love comic books and generally read your blog after school, while 20% are adults who enjoy sci-fi and who visit during the weekends. If you use a *hierarchical clustering* algorithm, it may also subdivide each group into smaller groups. This may help you target your posts for each group.

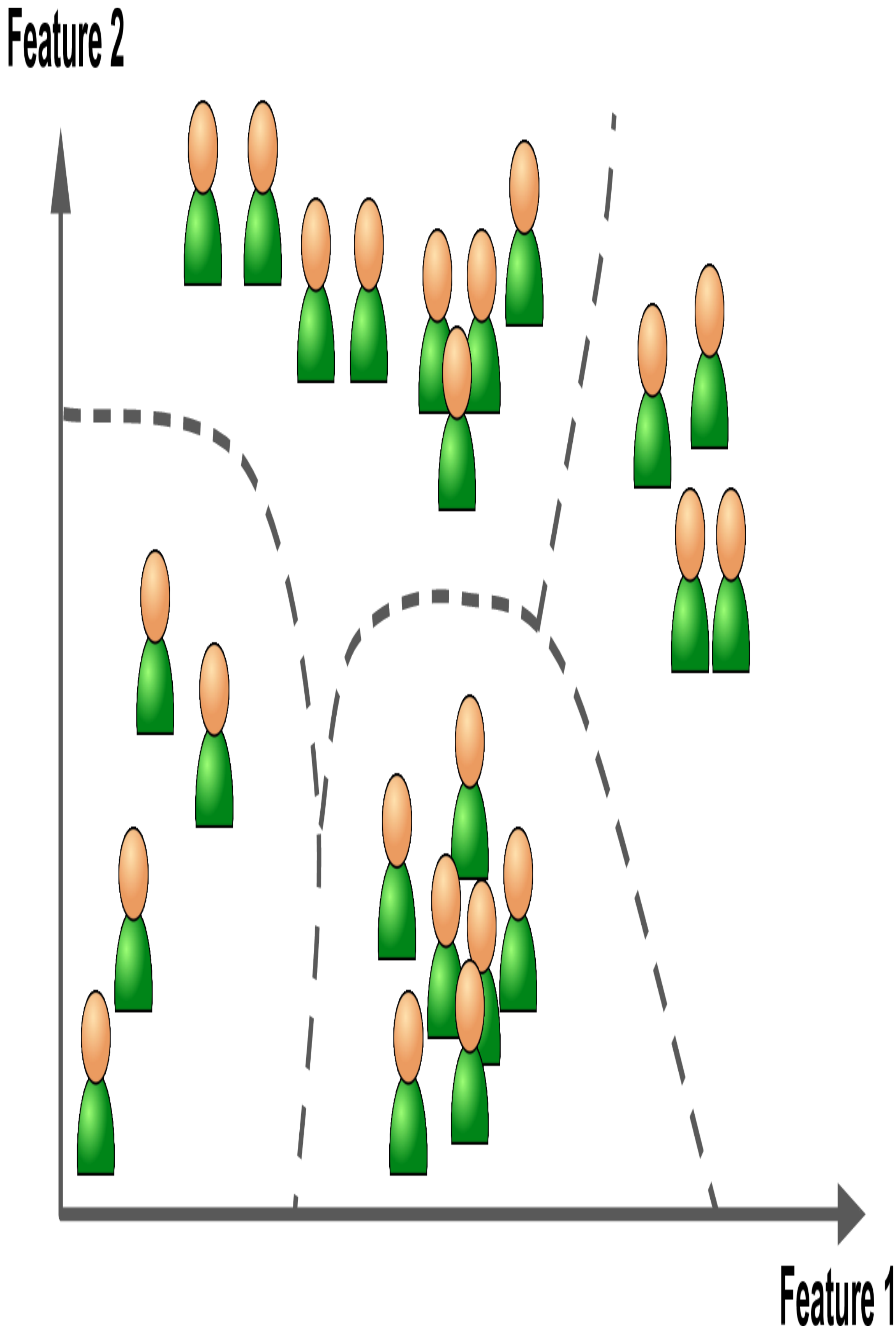

Feature 2
Feature 1

Figure 1-8. Clustering

Visualization algorithms are also good examples of unsupervised learning: you feed them a lot of complex and unlabeled data, and they output a 2D or 3D representation of your data that can easily be plotted (Figure 1-9). These algorithms try to preserve as much structure as they can (e.g., trying to keep separate clusters in the input space from overlapping in the visualization) so that you can understand how the data is organized and perhaps identify unsuspected patterns.

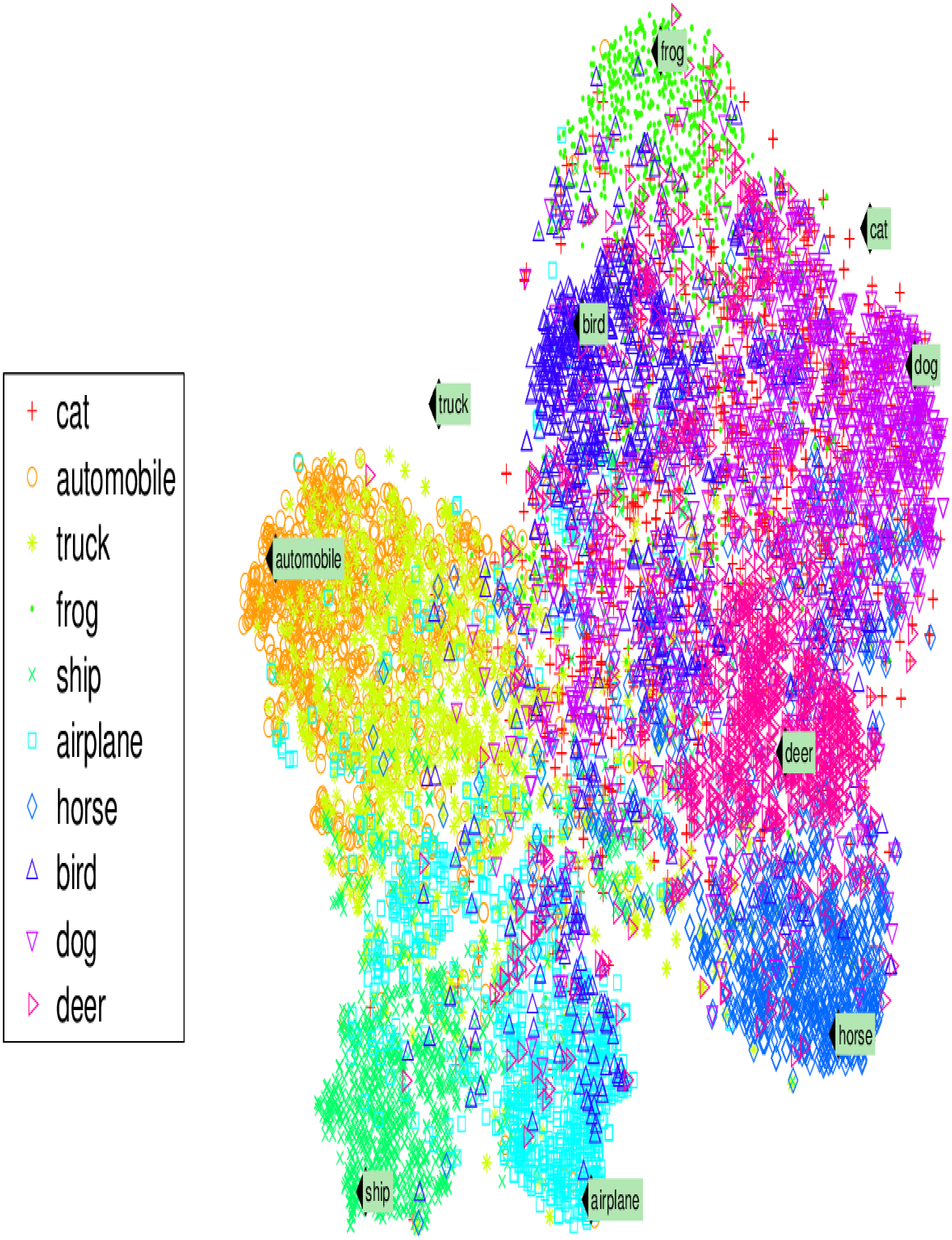


Figure 1-9. Example of a t-SNE visualization highlighting semantic clusters[2]

A related task is *dimensionality reduction*, in which the goal is to simplify the data without losing too much information. One way to do this is to merge several correlated features into one. For example, a car's mileage may be strongly correlated with its age, so the dimensionality reduction algorithm will merge them into one feature that represents the car's wear and tear. This is called *feature extraction*.

> **TIP**
>
> It is often a good idea to try to reduce the dimension of your training data using a dimensionality reduction algorithm before you feed it to another Machine Learning algorithm (such as a supervised learning algorithm). It will run much faster, the data will take up less disk and memory space, and in some cases it may also perform better.

Yet another important unsupervised task is *anomaly detection*—for example, detecting unusual credit card transactions to prevent fraud, catching manufacturing defects, or automatically removing outliers from a dataset before feeding it to another learning algorithm. The system is shown mostly normal instances during training, so it learns to recognize them; then, when it sees a new instance, it can tell whether it looks like a normal one or whether it is likely an anomaly (see Figure 1-10). A very similar task is *novelty detection*: it aims to detect new instances that look different from all instances in the training set. This requires having a very "clean" training set, devoid of any instance that you would like the algorithm to detect. For example, if you have thousands of pictures of dogs, and 1% of these pictures represent Chihuahuas, then a novelty detection algorithm should not treat new pictures of Chihuahuas as novelties. On the other hand, anomaly detection algorithms may consider these dogs as so rare and so different from other dogs that they would likely classify them as anomalies (no offense to Chihuahuas).

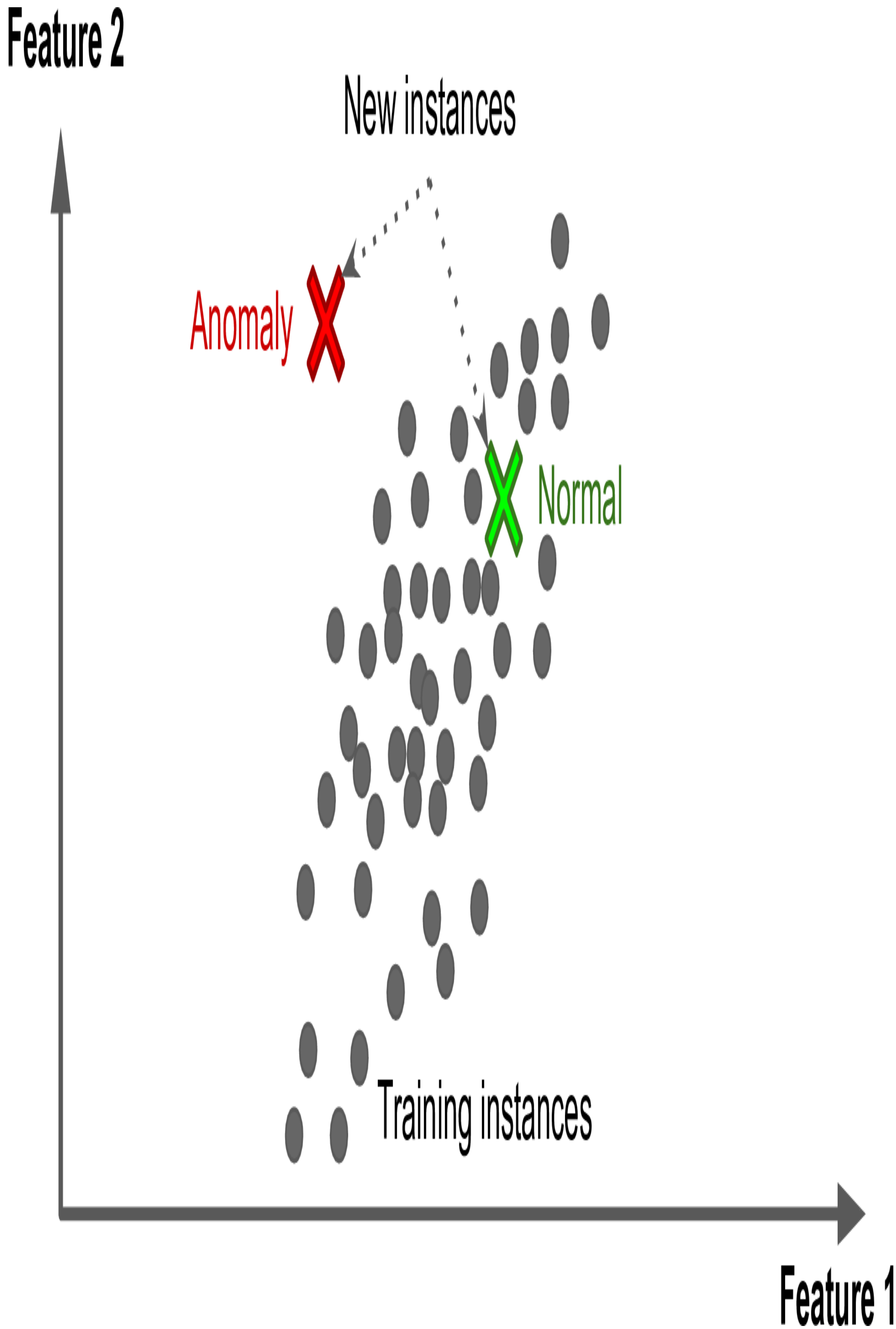
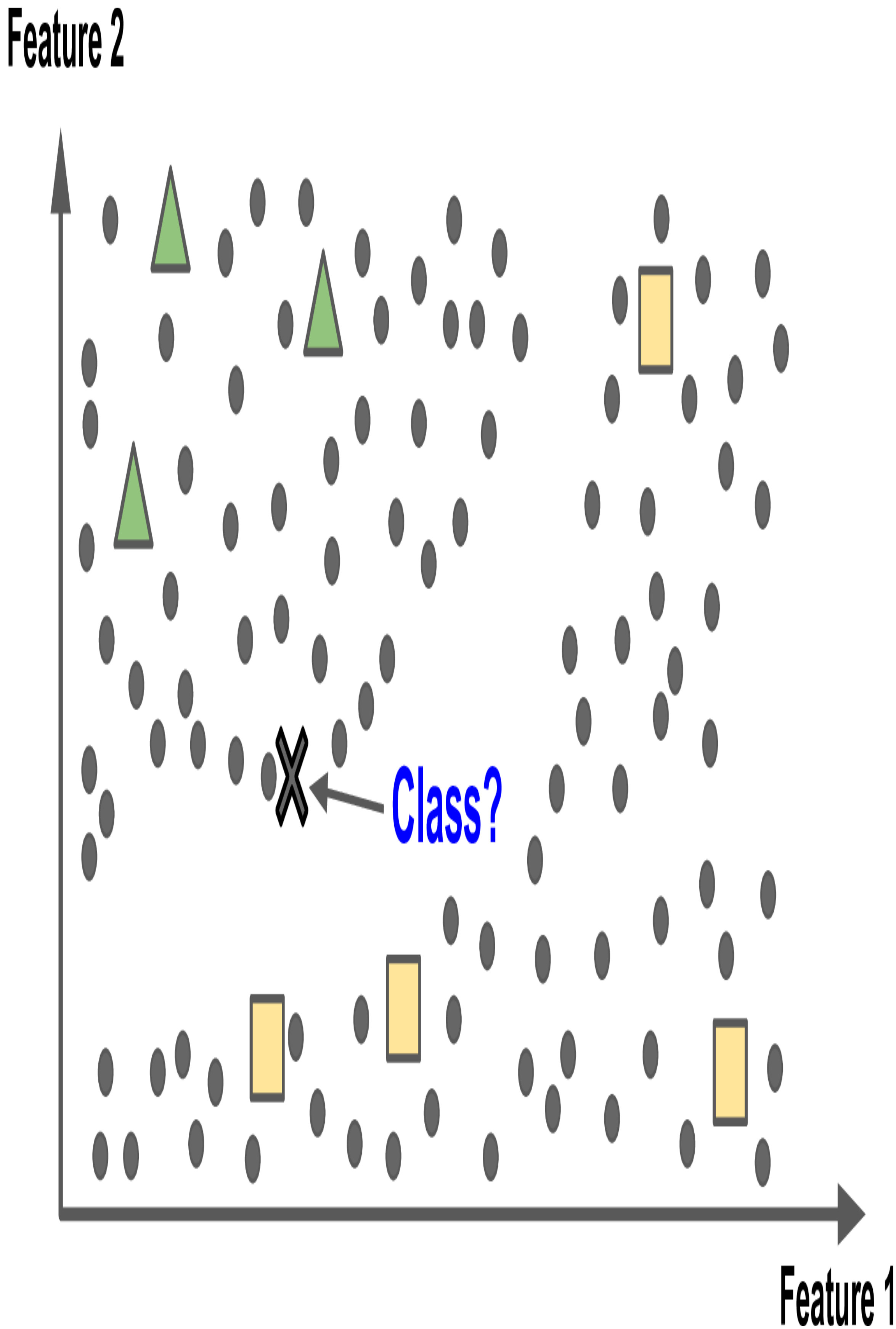

Feature 2
New instances
Anomaly
Normal
Training instances
Feature 1

Figure 1-10. Anomaly detection

Finally, another common unsupervised task is *association rule learning*, in which the goal is to dig into large amounts of data and discover interesting relations between attributes. For example, suppose you own a supermarket. Running an association rule on your sales logs may reveal that people who purchase barbecue sauce and potato chips also tend to buy steak. Thus, you may want to place these items close to one another.

Semi-supervised learning

Since labeling data is usually time-consuming and costly, you will often have plenty of unlabeled instances, and few labeled instances. Some algorithms can deal with data that's partially labeled. This is called *semi-supervised learning* (Figure 1-11).



Feature 2
Class?
Feature 1

Figure 1-11. Semi-supervised learning with two classes (triangles and squares): the unlabeled examples (circles) help classify a new instance (the cross) into the triangle class rather than the square class, even though it is closer to the labeled squares

Some photo-hosting services, such as Google Photos, are good examples of this. Once you upload all your family photos to the service, it automatically recognizes that the same person A shows up in photos 1, 5, and 11, while another person B shows up in photos 2, 5, and 7. This is the unsupervised part of the algorithm (clustering). Now all the system needs is for you to tell it who these people are. Just add one label per person[3] and it is able to name everyone in every photo, which is useful for searching photos.

Most semi-supervised learning algorithms are combinations of unsupervised and supervised algorithms. For example a clustering algorithm may be used to group similar instances together, and then every unlabeled instance can be labeled with the most common label in their cluster. Once the whole dataset is labeled, it is possible to use any supervised learning algorithm.

Self-supervised learning

Another approach to Machine Learning involves actually generating a fully labeled dataset from a fully unlabeled one. Again, once the whole dataset it labeled, any supervised learning algorithm can be used. This approach is called *self-supervised learning*.

For example, if you have a large dataset of unlabeled images, you can randomly mask a small part of each image and then train a model to recover the original image (Figure 1-12). During training, the masked images are used as the inputs to the model, and the original images are used as the labels.

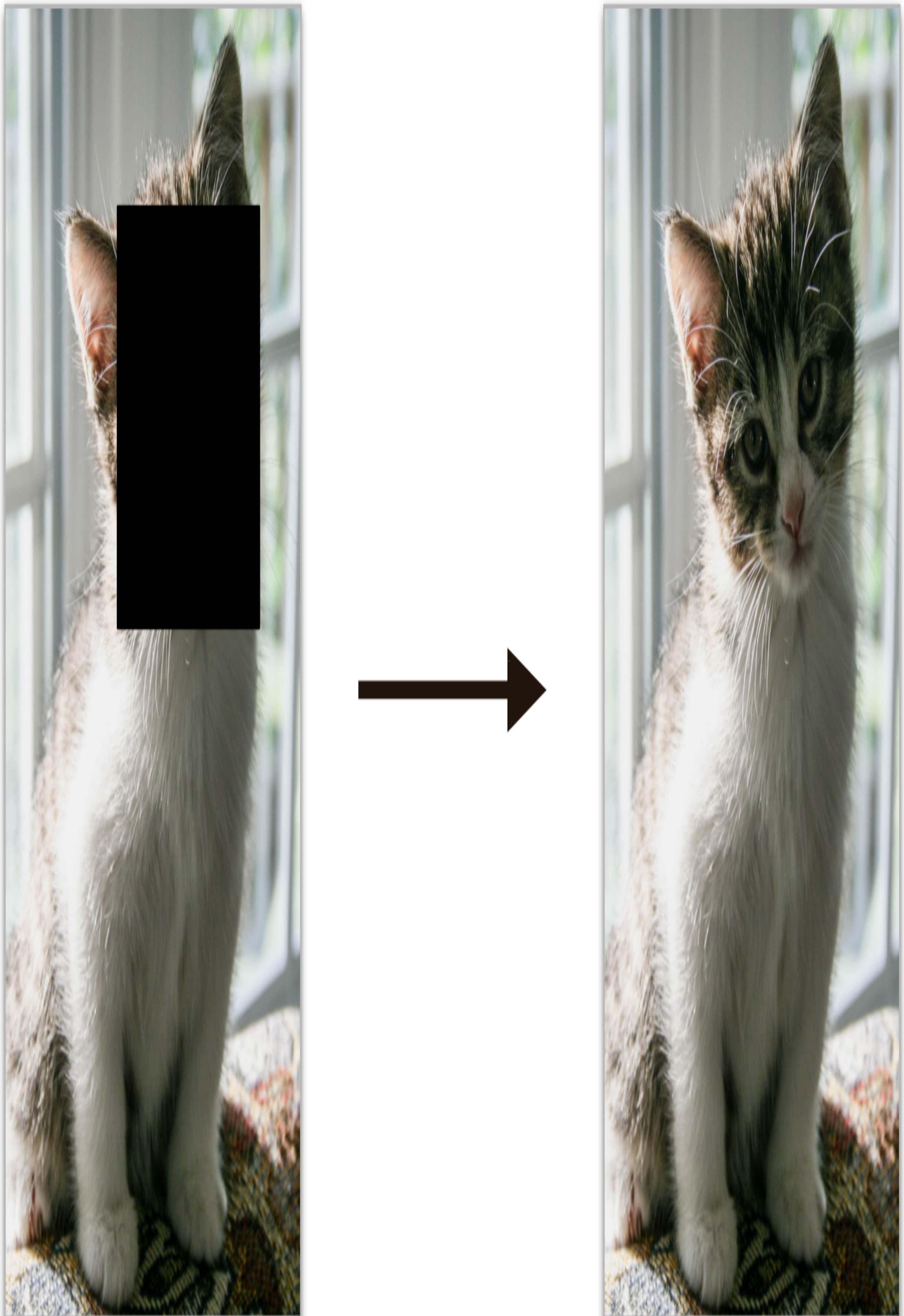


Figure 1-12. Self-supervised learning example: input (left) and target (right)

The resulting model may be quite useful in itself, for example to repair damaged images or to erase unwanted objects from pictures. But more often than not, a model trained using self-supervised learning is not the final goal. You usually want to tweak and fine-tune the model for a slightly different task. One that you actually care about.

For example, suppose that what you really want is to have a pet classification model: given a picture of any pet, it will tell you what species it belongs to. If you have a large dataset of unlabeled photos of pets, you can start by training an image-repairing model using self-supervised learning. Once it performs well, it must be able to distinguish different pet species: indeed, when it repairs an image of a cat whose face is masked, it knows it must not add a dog's face. Assuming your model's architecture allows it (and most neural network architectures do), it is then possible to tweak the model so that it predicts pet species instead of repairing images. The final step consists of fine-tuning the model on a labeled dataset: the model already knows what cats, dogs and other pet species look like, so this step is only needed so the model can learn the mapping between the species it already knows and the labels we expect from it.

NOTE

Transferring knowledge from one task to another is called *transfer learning*, and it's one of the most important techniques in Machine Learning today, especially when using *deep neural networks* (i.e., neural networks composed of many layers of neurons). We will discuss this in detail in Part II.

Some people consider self-supervised learning to be a part of unsupervised learning, since it deals with fully unlabeled datasets. But self-supervised learning uses (generated) labels during training, so in that regard it's closer to supervised learning. And the term "unsupervised learning" is generally used when dealing with tasks like clustering, dimensionality reduction or anomaly detection, whereas self-supervised learning focuses on the same tasks as supervised learning: mainly classification and regression. In short, it’s best to treat self-supervised learning as its own category.

Reinforcement Learning

Reinforcement Learning is a very different beast. The learning system, called an *agent* in this context, can observe the environment, select and perform actions, and get *rewards* in return (or *penalties* in the form of negative rewards, as shown in Figure 1-13). It must then learn by itself what is the best strategy, called a *policy*, to get the most reward over time. A policy defines what action the agent should choose when it is in a given situation.

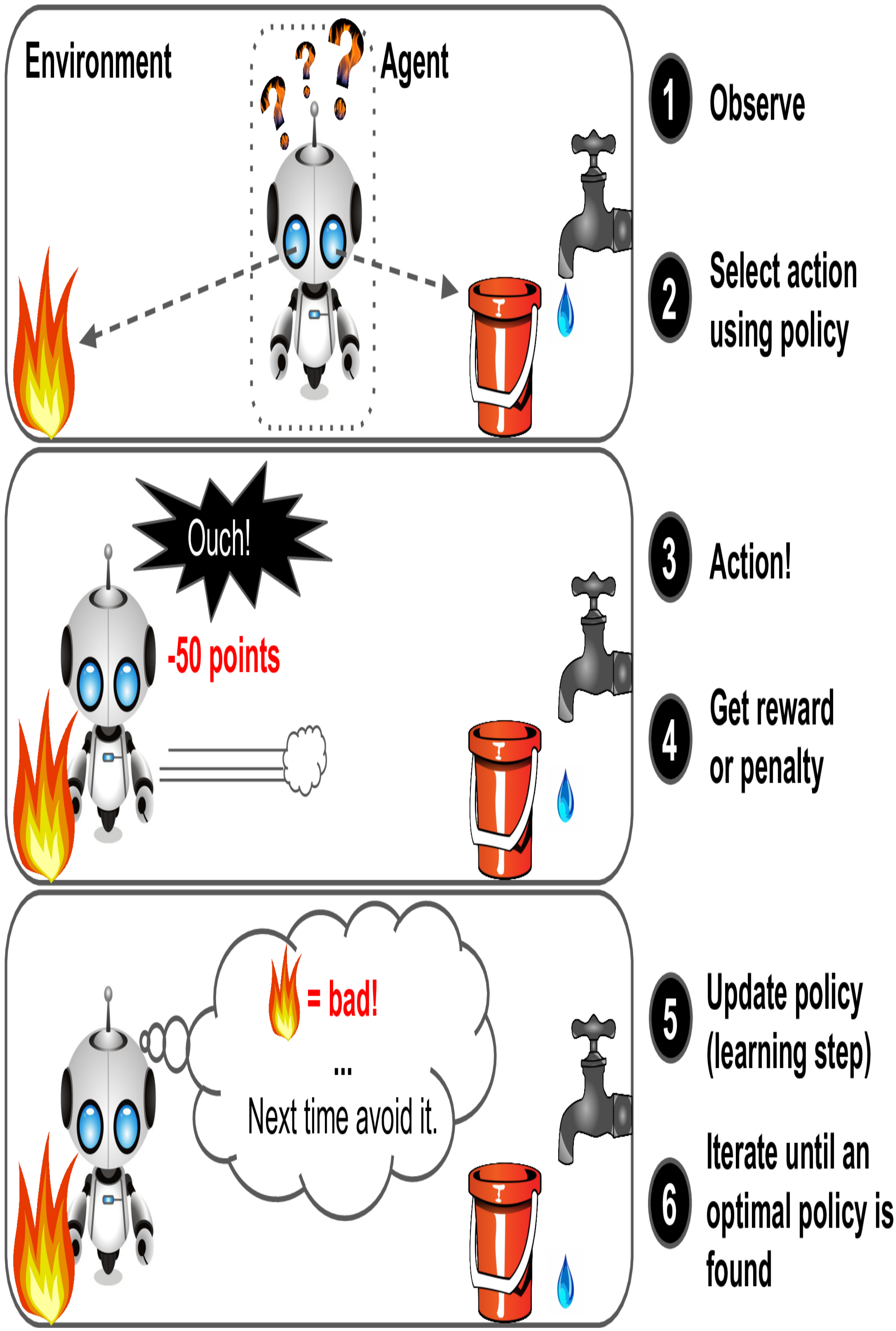

Environment
Agent
1 Observe
2 Select action using policy
Ouch!
-50 points
3 Action!
4 Get reward or penalty
= bad!
...
Next time avoid it.
5 Update policy (learning step)
6 Iterate until an optimal policy is found

Figure 1-13. Reinforcement Learning

For example, many robots implement Reinforcement Learning algorithms to learn how to walk. DeepMind's AlphaGo program is also a good example of Reinforcement Learning: it made the headlines in May 2017 when it beat Ke Jie, the number one ranked player in the world at the time, at the game of Go. It learned its winning policy by analyzing millions of games, and then playing many games against itself. Note that learning was turned off during the games against the champion; AlphaGo was just applying the policy it had learned. As we will see in the next section, this is called *offline learning*.

Batch versus Online Learning

Another criterion used to classify Machine Learning systems is whether or not the system can learn incrementally from a stream of incoming data.

Batch learning

In *batch learning*, the system is incapable of learning incrementally: it must be trained using all the available data. This will generally take a lot of time and computing resources, so it is typically done offline. First the system is trained, and then it is launched into production and runs without learning anymore; it just applies what it has learned. This is called *offline learning*.

Unfortunately, a model's performance tends to decay slowly over time, simply because the world continues to evolve while the model remains unchanged. This phenomenon is often called *model rot* or *data drift*. The solution is to regularly retrain the model on up-to-date data. How often you need to do that depends on the use case: if the model classifies pictures of cats and dogs, its performance will decay very slowly, but if the model deals with fast-evolving systems, for example making predictions on the financial market, then it is likely to decay quite fast.

WARNING

Even a model trained to classify pictures of cats and dogs may need to be retrained regularly, not because cats and dogs will mutate overnight, but because cameras keep changing, along with image formats, sharpness, brightness, and size ratios. Moreover, people may love different breeds next year, or they may decide to dress their pets with tiny hats—who knows?

If you want a batch learning system to know about new data (such as a new type of spam), you need to train a new version of the system from scratch on the full dataset (not just the new data, but also the old data), then replace the old model with the new one. Fortunately, the whole process of training, evaluating, and launching a Machine Learning system can be automated fairly easily (as we saw in Figure 1-3), so even a batch learning system can adapt to change. Simply update the data and train a new version of the system from scratch as often as needed.

This solution is simple and often works fine, but training using the full set of data can take many hours, so you would typically train a new system only every 24 hours or even just weekly. If your system needs to adapt to rapidly changing data (e.g., to predict stock prices), then you need a more reactive solution.

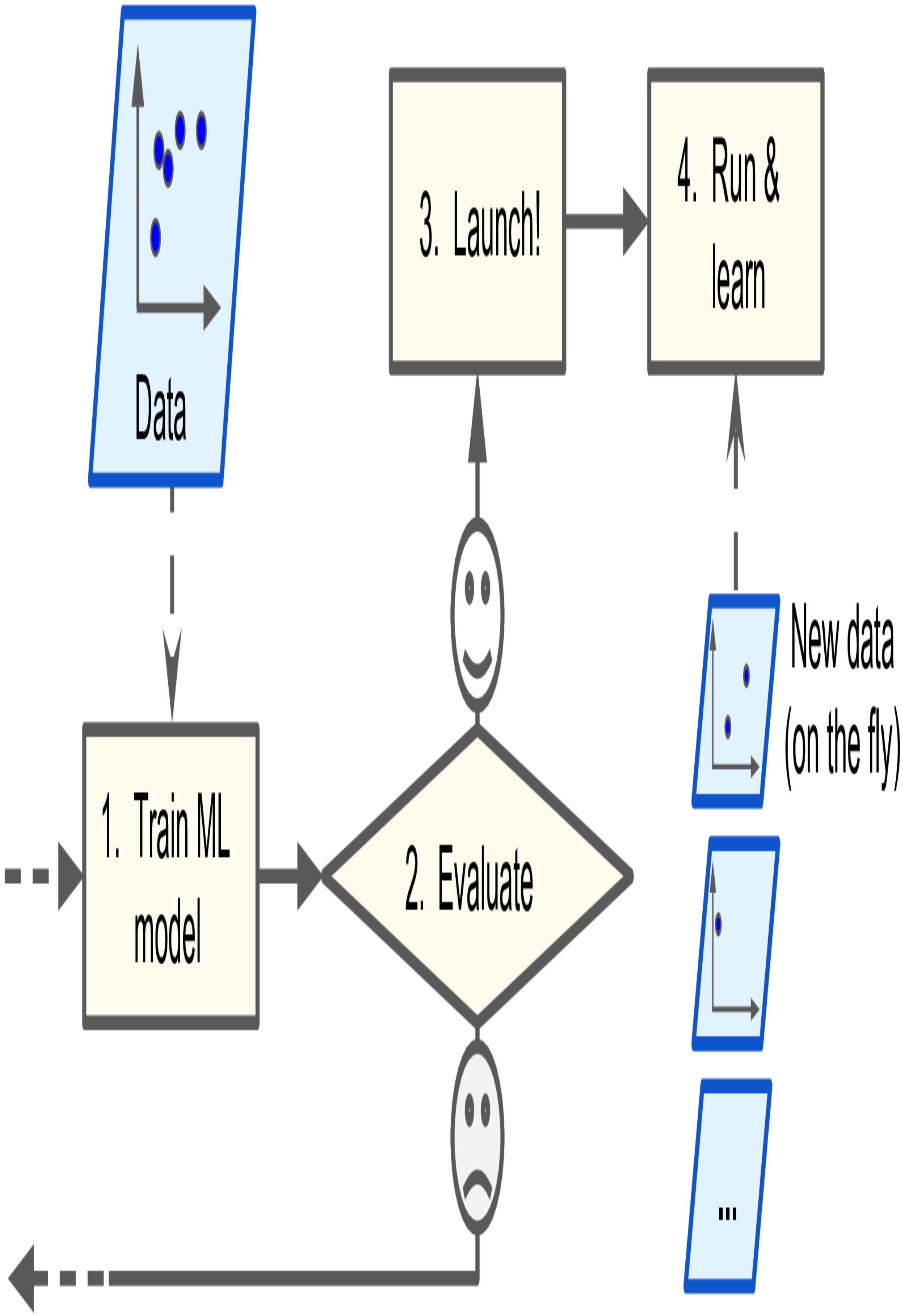
Also, training on the full set of data requires a lot of computing resources (CPU, memory space, disk space, disk I/O, network I/O, etc.). If you have a lot of data and you automate your system to train from scratch every day, it will end up costing you a lot of money. If the amount of data is huge, it may even be impossible to use a batch learning algorithm.

Finally, if your system needs to be able to learn autonomously and it has limited resources (e.g., a smartphone application or a rover on Mars), then carrying around large amounts of training data and taking up a lot of resources to train for hours every day is a showstopper.

Fortunately, a better option in all these cases is to use algorithms that are capable of learning incrementally.

Online learning

In *online learning*, you train the system incrementally by feeding it data instances sequentially, either individually or in small groups called *mini-batches*. Each learning step is fast and cheap, so the system can learn about new data on the fly, as it arrives (see Figure 1-14).



Data
3. Launch!
4. Run & learn
New data (on the fly)
...
1. Train ML model
2. Evaluate

Figure 1-14. In online learning, a model is trained and launched into production, and then it keeps learning as new data comes in

Online learning is useful for systems that need to adapt to change extremely rapidly (e.g., to detect new patterns in the stock market). It is also a good option if you have limited computing resources, for example if the model is trained on a mobile device.

Online learning algorithms can also be used to train models on huge datasets that cannot fit in one machine's main memory (this is called *out-of-core* learning). The algorithm loads part of the data, runs a training step on that data, and repeats the process until it has run on all of the data (see Figure 1-15).

WARNING

Out-of-core learning is usually done offline (i.e., not on the live system), so *online learning* can be a confusing name. Think of it as *incremental learning*.

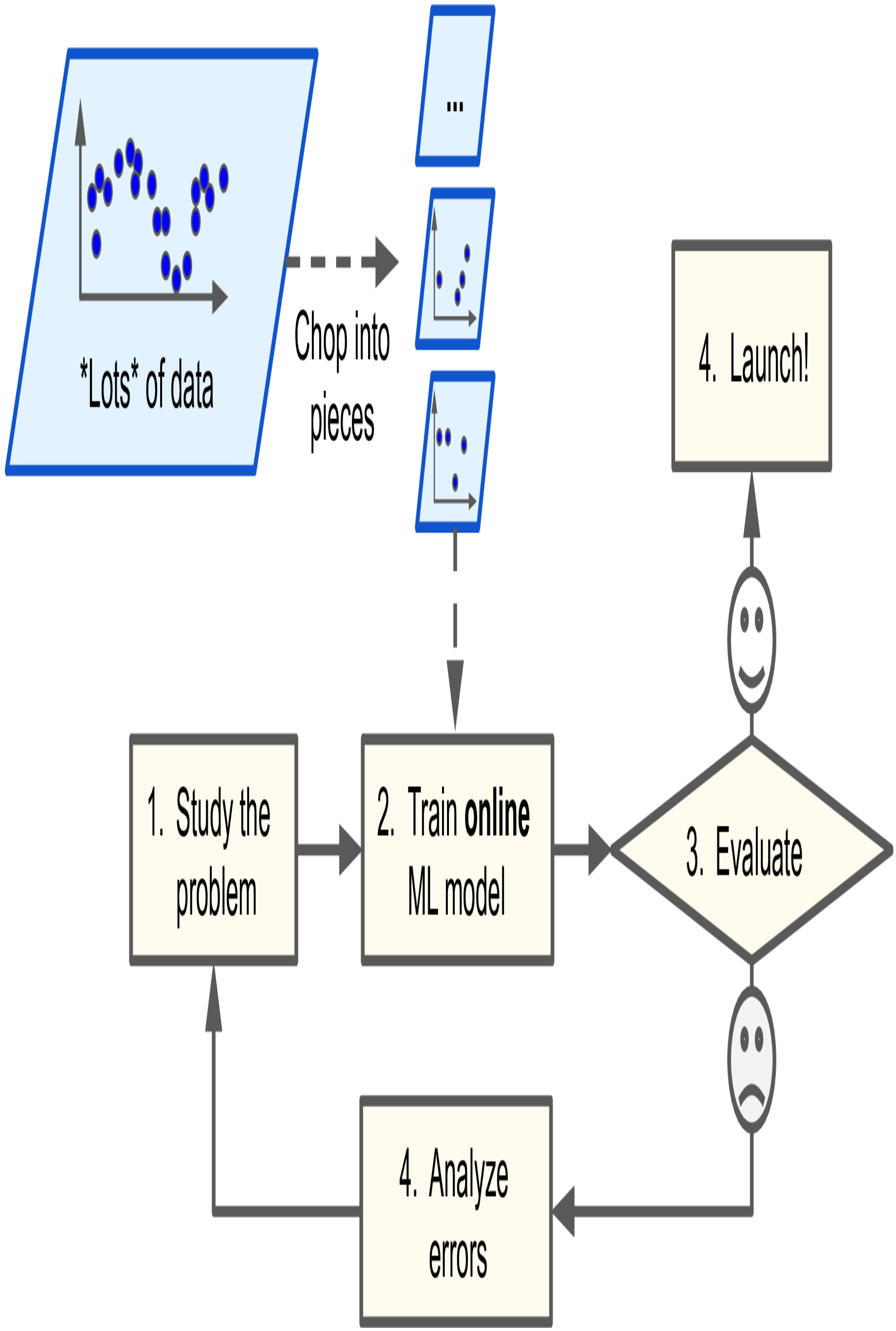

Lots of data
Chop into pieces
...
4. Launch!
1. Study the problem
2. Train **online** ML model
3. Evaluate
4. Analyze errors

Figure 1-15. Using online learning to handle huge datasets

One important parameter of online learning systems is how fast they should adapt to changing data: this is called the *learning rate*. If you set a high learning rate, then your system will rapidly adapt to new data, but it will also tend to quickly forget the old data (you don't want a spam filter to flag only the latest kinds of spam it was shown). Conversely, if you set a low learning rate, the system will have more inertia; that is, it will learn more slowly, but it will also be less sensitive to noise in the new data or to sequences of nonrepresentative data points (outliers).

A big challenge with online learning is that if bad data is fed to the system, the system's performance will decline, possibly quickly (depending on the data quality and learning rate). If it's a live system, your clients will notice. For example, bad data could come from a bug (e.g., a malfunctioning sensor on a robot), or it could come from someone trying to game the system (e.g., spamming a search engine to try to rank high in search results). To reduce this risk, you need to monitor your system closely and promptly switch learning off (and possibly revert to a previously working state) if you detect a drop in performance. You may also want to monitor the input data and react to abnormal data, for example using an anomaly detection algorithm (see Chapter 9).

Instance-Based Versus Model-Based Learning

One more way to categorize Machine Learning systems is by how they *generalize*. Most Machine Learning tasks are about making predictions. This means that given a number of training examples, the system needs to be able to make good predictions for (generalize to) examples it has never seen before. Having a good performance measure on the training data is good, but insufficient; the true goal is to perform well on new instances.

There are two main approaches to generalization: instance-based learning and model-based learning.

Instance-based learning

Possibly the most trivial form of learning is simply to learn by heart. If you were to create a spam filter this way, it would just flag all emails that are identical to emails that have already been flagged by users—not the worst solution, but certainly not the best.

Instead of just flagging emails that are identical to known spam emails, your spam filter could be programmed to also flag emails that are very similar to known spam emails. This requires a *measure of similarity* between two emails. A (very basic) similarity measure between two emails could be to count the number of words they have in common. The system would flag an email as spam if it has many words in common with a known spam email.

This is called *instance-based learning*: the system learns the examples by heart, then generalizes to new cases by using a similarity measure to compare them to the learned examples (or a subset of them). For example, in Figure 1-16 the new instance would be classified as a triangle because the majority of the most similar instances belong to that class.

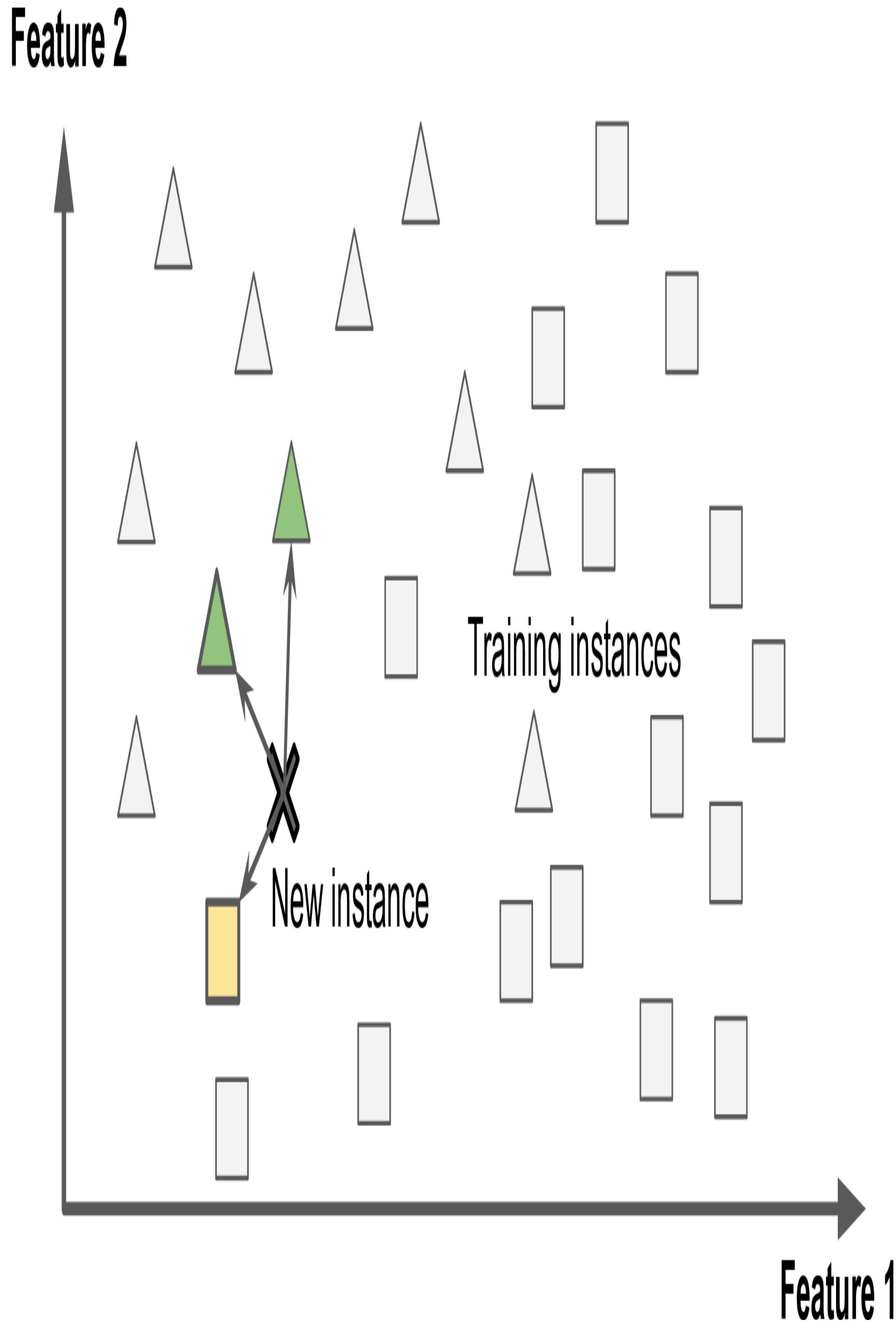

Feature 2
Training instances
New instance
Feature 1

Figure 1-16. Instance-based learning

Model-based learning, and a typical Machine Learning workflow

Another way to generalize from a set of examples is to build a model of these examples and then use that model to make *predictions*. This is called *model-based learning* (Figure 1-17).

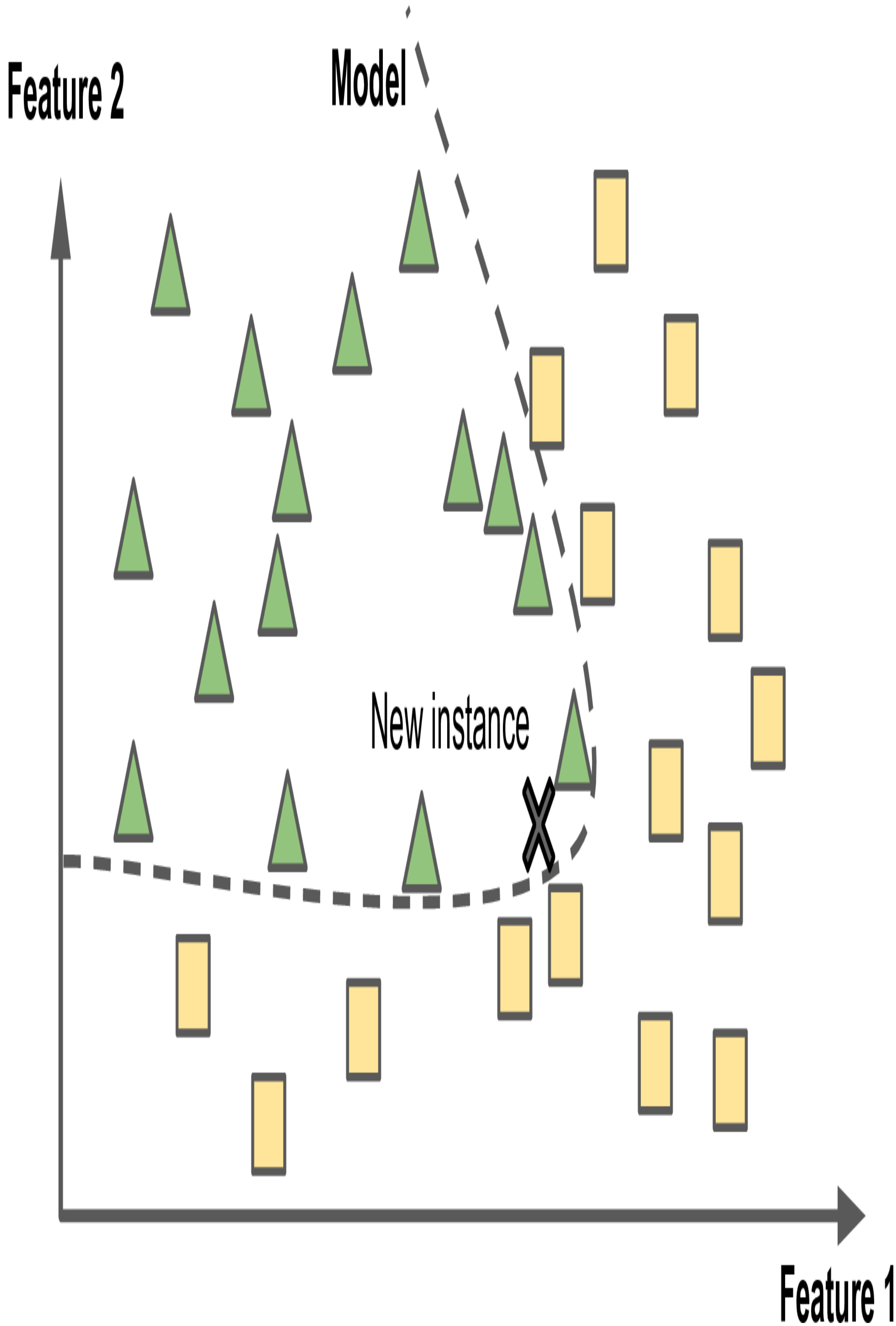

Model
Feature 2
New instance
Feature 1

Figure 1-17. Model-based learning

For example, suppose you want to know if money makes people happy, so you download the Better Life Index data from the OECD's website and World Bank stats about gross domestic product (GDP) per capita from OurWorldInData.org. Then you join the tables and sort by GDP per capita. Table 1-1 shows an excerpt of what you get.

Table 1-1. Does money make people ha

p
p
i
e
r
?

Country	GDP per capita (USD)	Life satisfaction
Turkey	28,384	5.5
Hungary	31,008	5.6
France	42,026	6.5
United States	60,236	6.9
New Zealand	42,404	7.3
Australia	48,698	7.3
Denmark	55,938	7.6

Let’s plot the data for these countries (Figure 1-18).

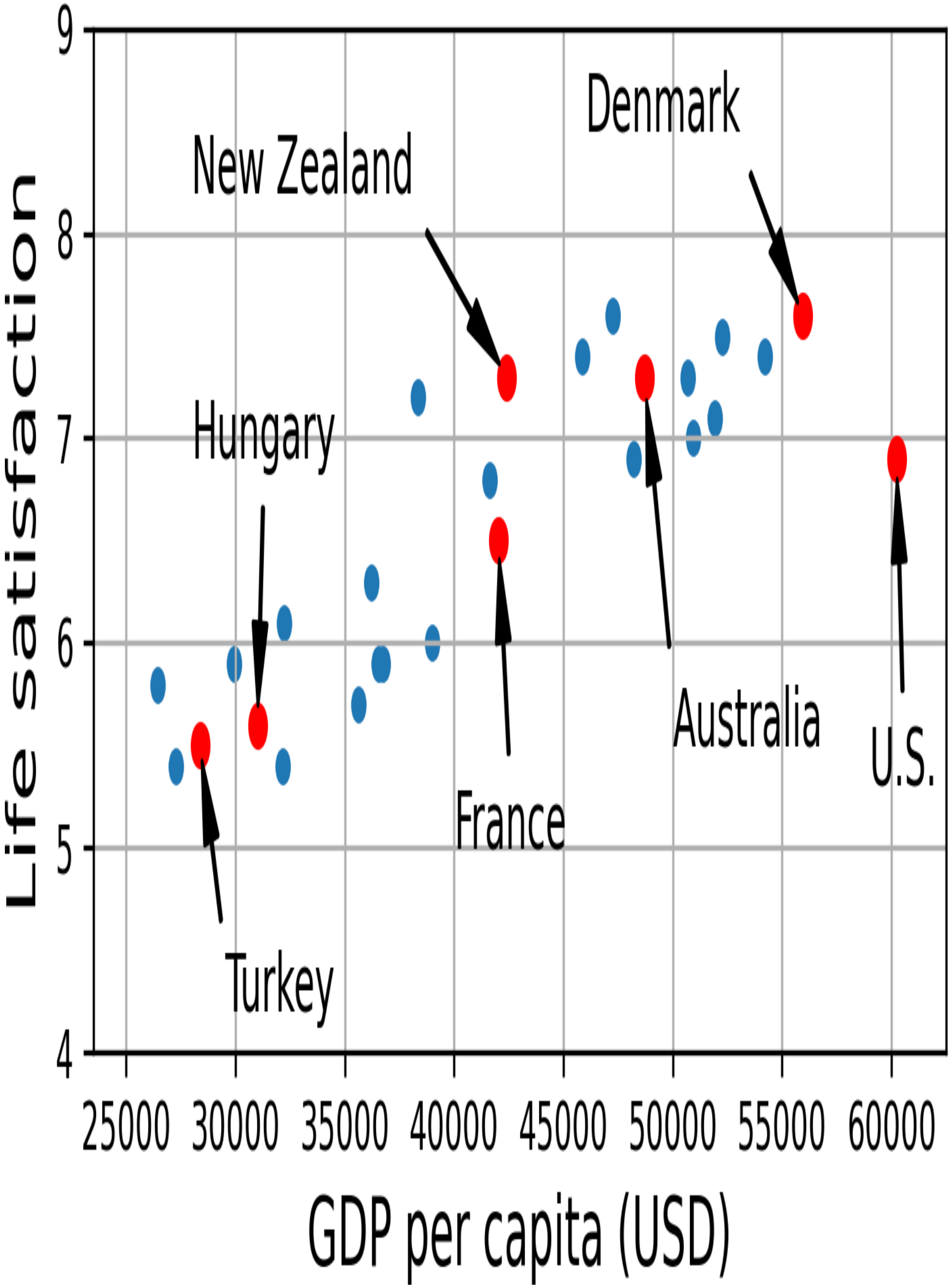


Figure 1-18. Do you see a trend here?

There does seem to be a trend here! Although the data is *noisy* (i.e., partly random), it looks like life satisfaction goes up more or less linearly as the country's GDP per capita increases. So you decide to model life satisfaction as a linear function of GDP per capita. This step is called *model selection*: you selected a *linear model* of life satisfaction with just one attribute, GDP per capita (Equation 1-1).

Equation 1-1. A simple linear model

$$\text{life\_satisfaction} = \theta_0 + \theta_1 \times \text{GDP\_per\_capita}$$

This model has two *model parameters*, θ_0 and θ_1.[4] By tweaking these parameters, you can make your model represent any linear function, as shown in Figure 1-19.

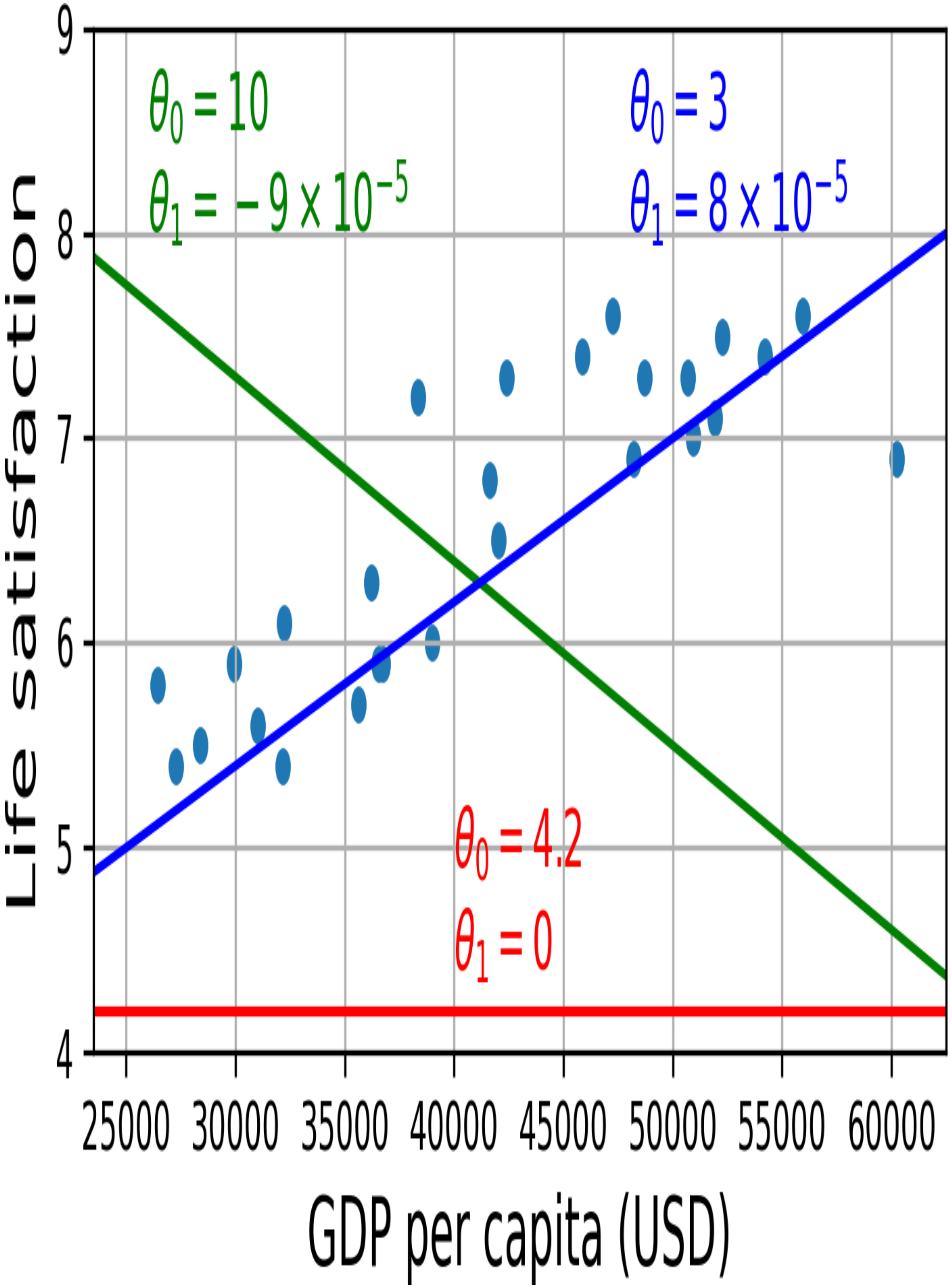


Figure 1-19. A few possible linear models

Before you can use your model, you need to define the parameter values θ_0 and θ_1. How can you know which values will make your model perform best? To answer this question, you need to specify a performance measure. You can either define a *utility function* (or *fitness function*) that measures how *good* your model is, or you can define a *cost function* that measures how *bad* it is. For Linear Regression problems, people typically use a cost function that measures the distance between the linear model's predictions and the training examples; the objective is to minimize this distance.

This is where the Linear Regression algorithm comes in: you feed it your training examples, and it finds the parameters that make the linear model fit best to your data. This is called *training* the model. In our case, the algorithm finds that the optimal parameter values are $\theta_0 = 3.75$ and $\theta_1 = 6.78 \times 10^{-5}$.

WARNING

Confusingly, the same word "model" can refer to a *type of model* (e.g., Linear Regression), to a *fully specified model architecture* (e.g., Linear Regression with one input and one output), or to the *final trained model* ready to be used for predictions (e.g., Linear Regression with one input and one output, using $\theta_0 = 3.75$ and $\theta_1 = 6.78 \times 10^{-5}$). Model selection consists in choosing the type of model and fully specifying its architecture. Training a model means running an algorithm to find the model parameters that will make it best fit the training data, and hopefully make good predictions on new data.

Now the model fits the training data as closely as possible (for a linear model), as you can see in Figure 1-20.

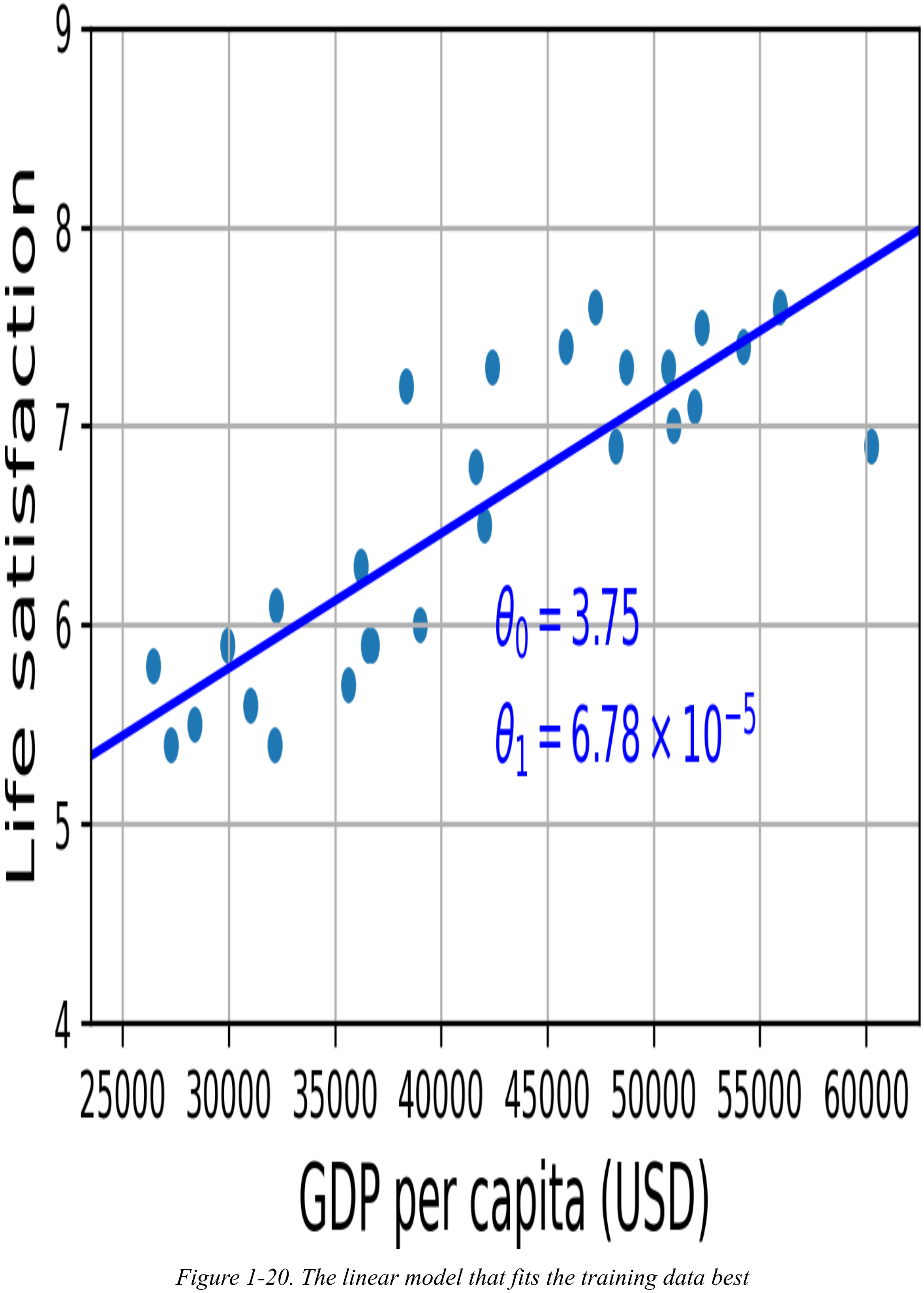


Figure 1-20. The linear model that fits the training data best

You are finally ready to run the model to make predictions. For example, say you want to know how happy Cypriots are, and the OECD data does not have the answer. Fortunately, you can use your model to make a good prediction: you look up Cyprus's GDP per capita, find $37,655, and then apply your model and find that life satisfaction is likely to be somewhere around $3.75 + 37{,}655 \times 6.78 \times 10^{-5} = 6.30$.

To whet your appetite, Example 1-1 shows the Python code that loads the data, separates the inputs `X` from the labels `y`, creates a scatterplot for visualization, and then trains a linear model and makes a prediction.[5]

Example 1-1. Training and running a linear model using Scikit-Learn

```
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
from sklearn.linear_model import LinearRegression

# Download and prepare the data
data_root = "https://github.com/ageron/data/raw/main/"
lifesat = pd.read_csv(data_root + "lifesat/lifesat.csv")
X = lifesat[["GDP per capita (USD)"]].values
y = lifesat[["Life satisfaction"]].values

# Visualize the data
lifesat.plot(kind='scatter', grid=True,
             x="GDP per capita (USD)", y="Life satisfaction")
plt.axis([23_500, 62_500, 4, 9])
plt.show()

# Select a linear model
model = LinearRegression()

# Train the model
model.fit(X, y)

# Make a prediction for Cyprus
X_new = [[37_655.2]]  # Cyprus' GDP per capita in 2020
print(model.predict(X_new)) # outputs [[6.30165767]]
```

NOTE

If you had used an instance-based learning algorithm instead, you would have found that Israel has the closest GDP per capita to that of Cyprus ($38,341), and since the OECD data tells us that Israelis' life satisfaction is 7.2, you would have predicted a life satisfaction of 7.2 for Cyprus. If you zoom out a bit and look at the two next-closest countries, you will find Lithuania and Slovenia, both with a life satisfaction of 5.9. Averaging these three values, you get 6.33, which is pretty close to your model-based prediction. This simple algorithm is called *k-Nearest Neighbors* regression (in this example, $k = 3$).

Replacing the Linear Regression model with k-Nearest Neighbors regression in the previous code is as simple as replacing these two lines:

```
from sklearn.linear_model import LinearRegression
model = LinearRegression()
```

with these two:

```
from sklearn.neighbors import KNeighborsRegressor
model = KNeighborsRegressor(n_neighbors=3)
```

If all went well, your model will make good predictions. If not, you may need to use more attributes (employment rate, health, air pollution, etc.), get more or better-quality training data, or perhaps select a more powerful model (e.g., a Polynomial Regression model).

In summary:

- You studied the data.
- You selected a model.
- You trained it on the training data (i.e., the learning algorithm searched for the model parameter values that minimize a cost function).
- Finally, you applied the model to make predictions on new cases (this is called *inference*), hoping that this model will generalize well.

This is what a typical Machine Learning project looks like. In Chapter 2 you will experience this firsthand by going through a project end to end.

We have covered a lot of ground so far: you now know what Machine Learning is really about, why it is useful, what some of the most common categories of ML systems are, and what a typical project workflow looks like. Now let's look at what can go wrong in learning and prevent you from making accurate predictions.

Main Challenges of Machine Learning

In short, since your main task is to select a model and train it on some data, the two things that can go wrong are "bad model" and "bad data." Let's start with examples of bad data.

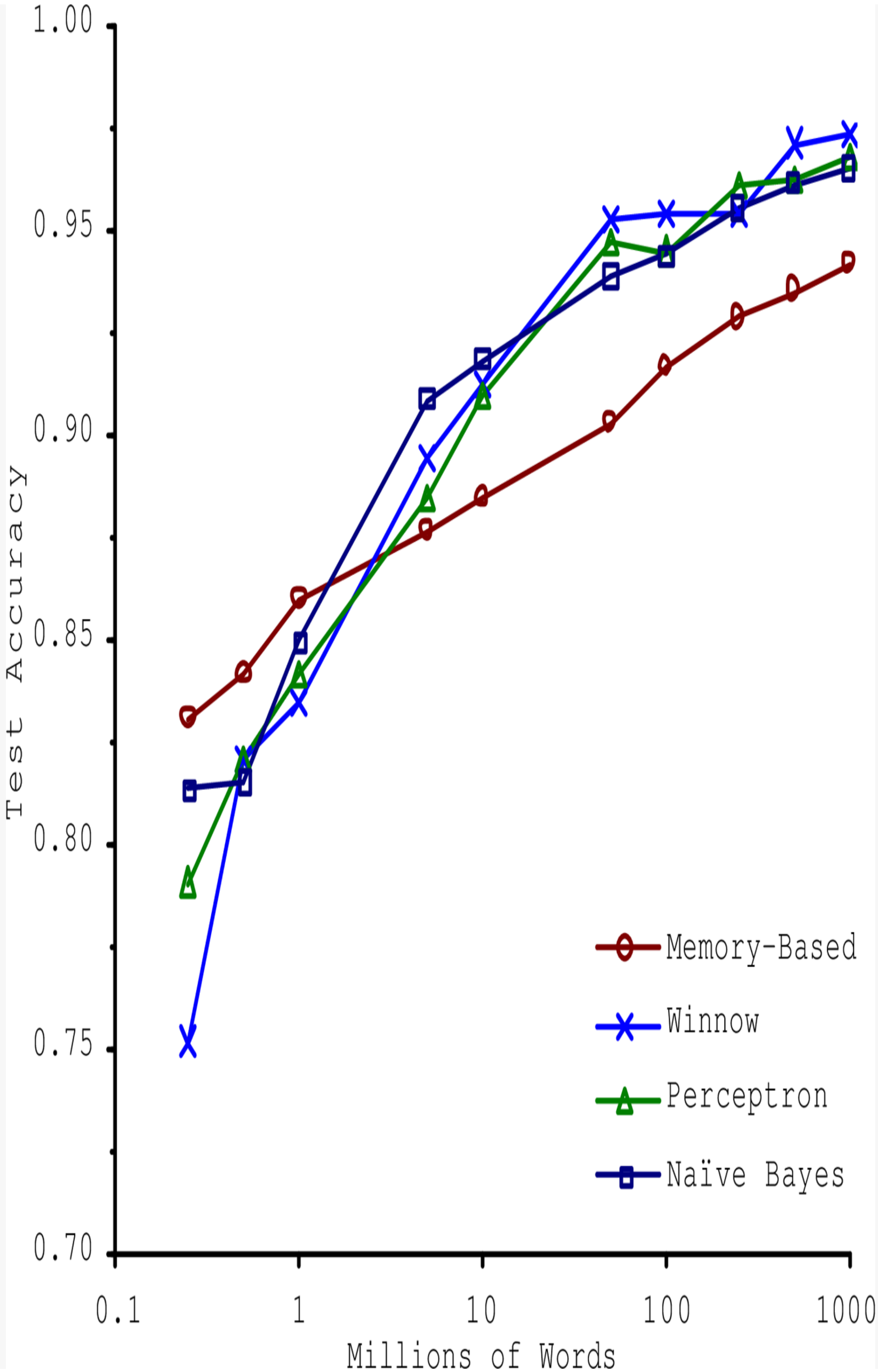
Insufficient Quantity of Training Data

For a toddler to learn what an apple is, all it takes is for you to point to an apple and say "apple" (possibly repeating this procedure a few times). Now the child is able to recognize apples in all sorts of colors and shapes. Genius.

Machine Learning is not quite there yet; it takes a lot of data for most Machine Learning algorithms to work properly. Even for very simple problems you typically need thousands of examples, and for complex problems such as image or speech recognition you may need millions of examples (unless you can reuse parts of an existing model).

THE UNREASONABLE EFFECTIVENESS OF DATA

In a famous paper published in 2001, Microsoft researchers Michele Banko and Eric Brill showed that very different Machine Learning algorithms, including fairly simple ones, performed almost identically well on a complex problem of natural language disambiguation[6] once they were given enough data (as you can see in Figure 1-21).



1.00
0.95
0.90
0.85
0.80
0.75
0.70
Test Accuracy
0.1
1
10
100
1000
Millions of Words
Memory-Based
Winnow
Perceptron
Naïve Bayes

Figure 1-21. The importance of data versus algorithms[7]

As the authors put it, “these results suggest that we may want to reconsider the trade-off between spending time and money on algorithm development versus spending it on corpus development.”

The idea that data matters more than algorithms for complex problems was further popularized by Peter Norvig et al. in a paper titled “The Unreasonable Effectiveness of Data”, published in 2009.[8] It should be noted, however, that small- and medium-sized datasets are still very common, and it is not always easy or cheap to get extra training data—so don’t abandon algorithms just yet.

Nonrepresentative Training Data

In order to generalize well, it is crucial that your training data be representative of the new cases you want to generalize to. This is true whether you use instance-based learning or model-based learning.

For example, the set of countries we used earlier for training the linear model was not perfectly representative; it did not contain any country with a GDP per capita lower than $23,500 or higher than $62,500. Figure 1-22 shows what the data looks like when you add such countries.

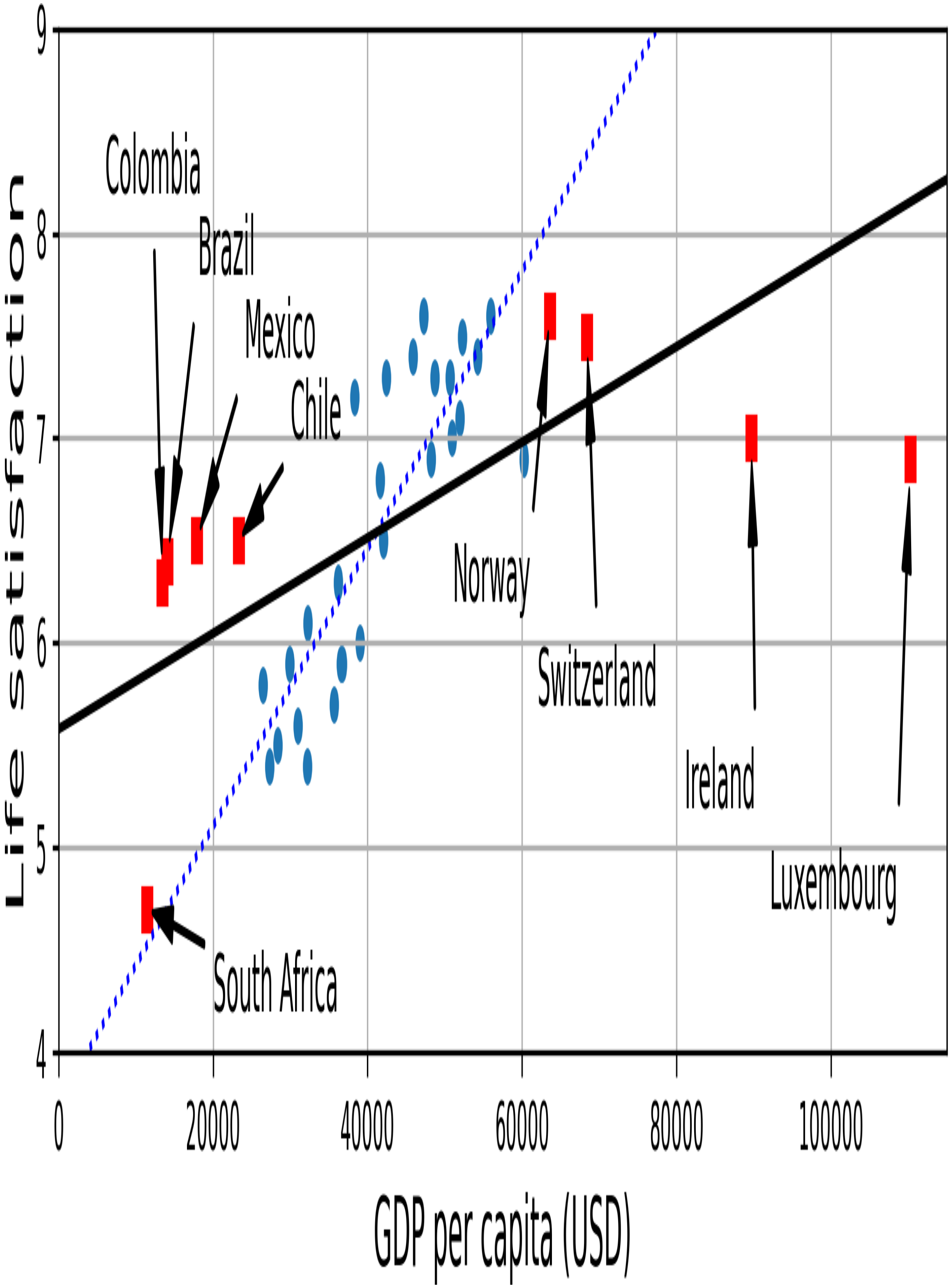


Figure 1-22. A more representative training sample

If you train a linear model on this data, you get the solid line, while the old model is represented by the dotted line. As you can see, not only does adding a few missing countries significantly alter the model, but it makes it clear that such a simple linear model is probably never going to work well. It seems that very rich countries are not happier than moderately rich countries (in fact, they seem slightly unhappier!), and conversely some poor countries seem happier than many rich countries.

By using a nonrepresentative training set, we trained a model that is unlikely to make accurate predictions, especially for very poor and very rich countries.

It is crucial to use a training set that is representative of the cases you want to generalize to. This is often harder than it sounds: if the sample is too small, you will have *sampling noise* (i.e., nonrepresentative data as a result of chance), but even very large samples can be nonrepresentative if the sampling method is flawed. This is called *sampling bias*.

EXAMPLES OF SAMPLING BIAS

Perhaps the most famous example of sampling bias happened during the US presidential election in 1936, which pitted Landon against Roosevelt: the *Literary Digest* conducted a very large poll, sending mail to about 10 million people. It got 2.4 million answers, and predicted with high confidence that Landon would get 57% of the votes. Instead, Roosevelt won with 62% of the votes. The flaw was in the *Literary Digest*'s sampling method:

- First, to obtain the addresses to send the polls to, the *Literary Digest* used telephone directories, lists of magazine subscribers, club membership lists, and the like. All of these lists tended to favor wealthier people, who were more likely to vote Republican (hence Landon).
- Second, less than 25% of the people who were polled answered. Again this introduced a sampling bias, by potentially ruling out people who didn't care much about politics, people who didn't like the *Literary Digest*, and other key groups. This is a special type of sampling bias called *nonresponse bias*.

Here is another example: say you want to build a system to recognize funk music videos. One way to build your training set is to search for "funk music" on YouTube and use the resulting videos. But this assumes that YouTube's search engine returns a set of videos that are representative of all the funk music videos on YouTube. In reality, the search results are likely to be biased toward popular artists (and if you live in Brazil you will get a lot of "funk carioca" videos, which sound nothing like James Brown). On the other hand, how else can you get a large training set?

Poor-Quality Data

Obviously, if your training data is full of errors, outliers, and noise (e.g., due to poor-quality measurements), it will make it harder for the system to detect the underlying patterns, so your system is less likely to perform well. It is often well worth the effort to spend time cleaning up your training data. The truth is, most data scientists spend a significant part of their time doing just that. The following are a couple examples of when you'd want to clean up training data:

- If some instances are clearly outliers, it may help to simply discard them or try to fix the errors manually.
- If some instances are missing a few features (e.g., 5% of your customers did not specify their age), you must decide whether you want to ignore this attribute altogether, ignore these instances, fill in the missing values (e.g., with the median age), or train one model with the feature and one model without it.

Irrelevant Features

As the saying goes: garbage in, garbage out. Your system will only be capable of learning if the training data contains enough relevant features and not too many irrelevant ones. A critical part of the success of a Machine Learning project is coming up with a good set of features to train on. This process, called *feature engineering*, involves the following steps:

- *Feature selection* (selecting the most useful features to train on among existing features)
- *Feature extraction* (combining existing features to produce a more useful one—as we saw earlier, dimensionality reduction algorithms can help)
- Creating new features by gathering new data

Now that we have looked at many examples of bad data, let's look at a couple examples of bad algorithms.

Overfitting the Training Data

Say you are visiting a foreign country and the taxi driver rips you off. You might be tempted to say that *all* taxi drivers in that country are thieves. Overgeneralizing is something that we humans do all too often, and unfortunately machines can fall into the same trap if we are not careful. In Machine Learning this is called *overfitting*: it means that the model performs well on the training data, but it does not generalize well.

Figure 1-23 shows an example of a high-degree polynomial life satisfaction model that strongly overfits the training data. Even though it performs much better on the training data than the simple linear model, would you really trust its predictions?

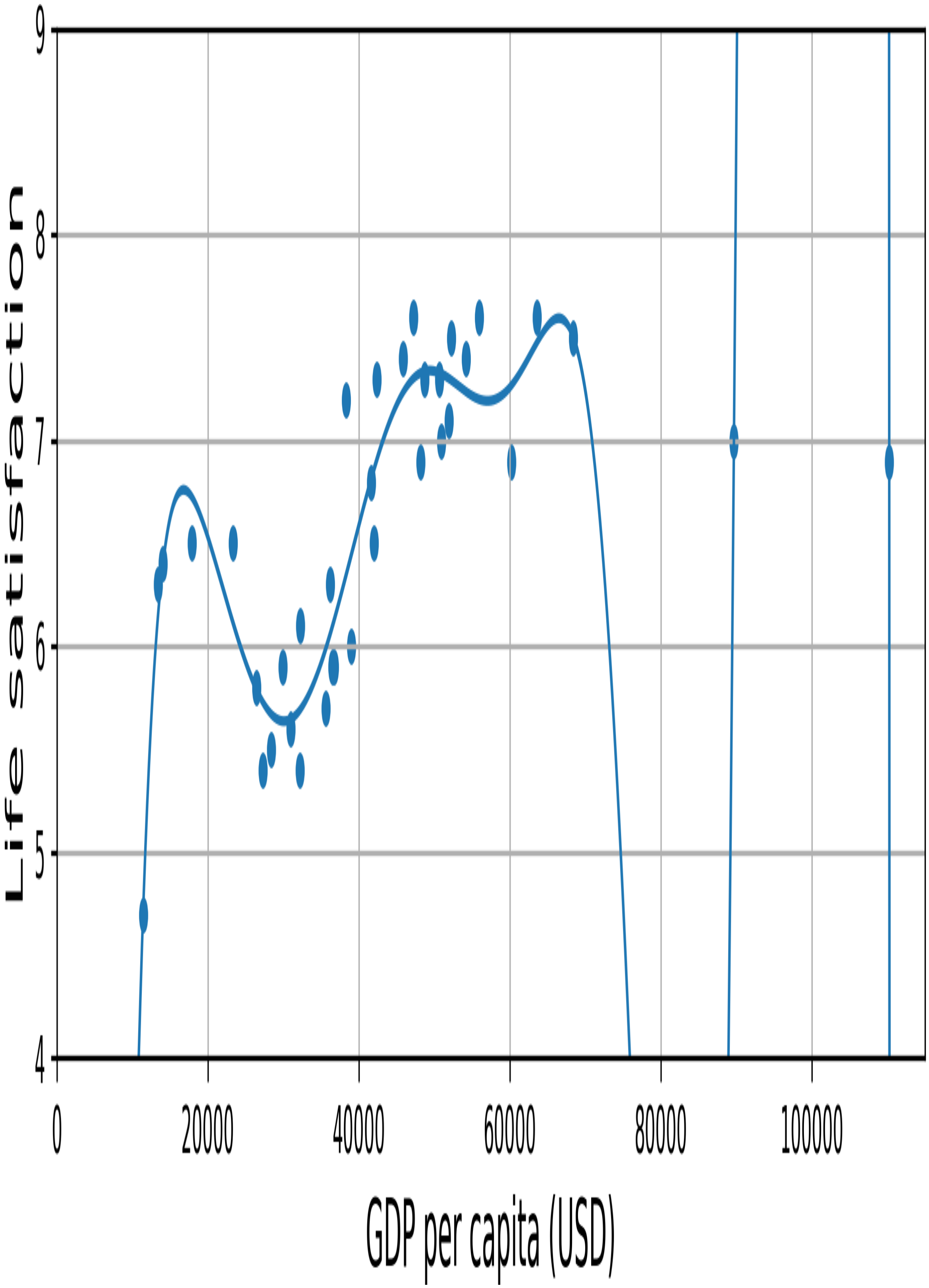


Figure 1-23. Overfitting the training data

Complex models such as deep neural networks can detect subtle patterns in the data, but if the training set is noisy, or if it is too small (which introduces sampling noise), then the model is likely to detect patterns in the noise itself. Obviously these patterns will not generalize to new instances. For example, say you feed your life satisfaction model many more attributes, including uninformative ones such as the country's name. In that case, a complex model may detect patterns like the fact that all countries in the training data with a *w* in their name have a life satisfaction greater than 7: New Zealand (7.3), Norway (7.6), Sweden (7.3), and Switzerland (7.5). How confident are you that the *w*-satisfaction rule generalizes to Rwanda or Zimbabwe? Obviously this pattern occurred in the training data by pure chance, but the model has no way to tell whether a pattern is real or simply the result of noise in the data.

WARNING

Overfitting happens when the model is too complex relative to the amount and noisiness of the training data. Here are possible solutions:

- Simplify the model by selecting one with fewer parameters (e.g., a linear model rather than a high-degree polynomial model), by reducing the number of attributes in the training data, or by constraining the model.
- Gather more training data.
- Reduce the noise in the training data (e.g., fix data errors and remove outliers).

Constraining a model to make it simpler and reduce the risk of overfitting is called *regularization*. For example, the linear model we defined earlier has two parameters, θ_0 and θ_1. This gives the learning algorithm two *degrees of freedom* to adapt the model to the training data: it can tweak both the height (θ_0) and the slope (θ_1) of the line. If we forced $\theta_1 = 0$, the algorithm would have only one degree of freedom and would have a much harder time fitting the data properly: all it could do is move the line up or down to get as close as possible to the training instances, so it would end up around the mean. A very simple model indeed! If we allow the algorithm to modify θ_1 but we force it to keep it small, then the learning algorithm will effectively have somewhere in between one and two degrees of freedom. It will produce a model that's simpler than one with two degrees of freedom, but more complex than one with just one. You want to find the right balance between fitting the training data perfectly and keeping the model simple enough to ensure that it will generalize well.

Figure 1-24 shows three models. The dotted line represents the original model that was trained on the countries represented as circles (without the countries represented as squares), the solid line is our second model trained with all countries (circles and squares), and the dashed line is a model trained with the same data as the first model but with a regularization constraint. You can see that regularization forced the model to have a smaller slope: this model does not fit the training data (circles) as well as the first model, but it actually generalizes better to new examples that it did not see during training (squares).

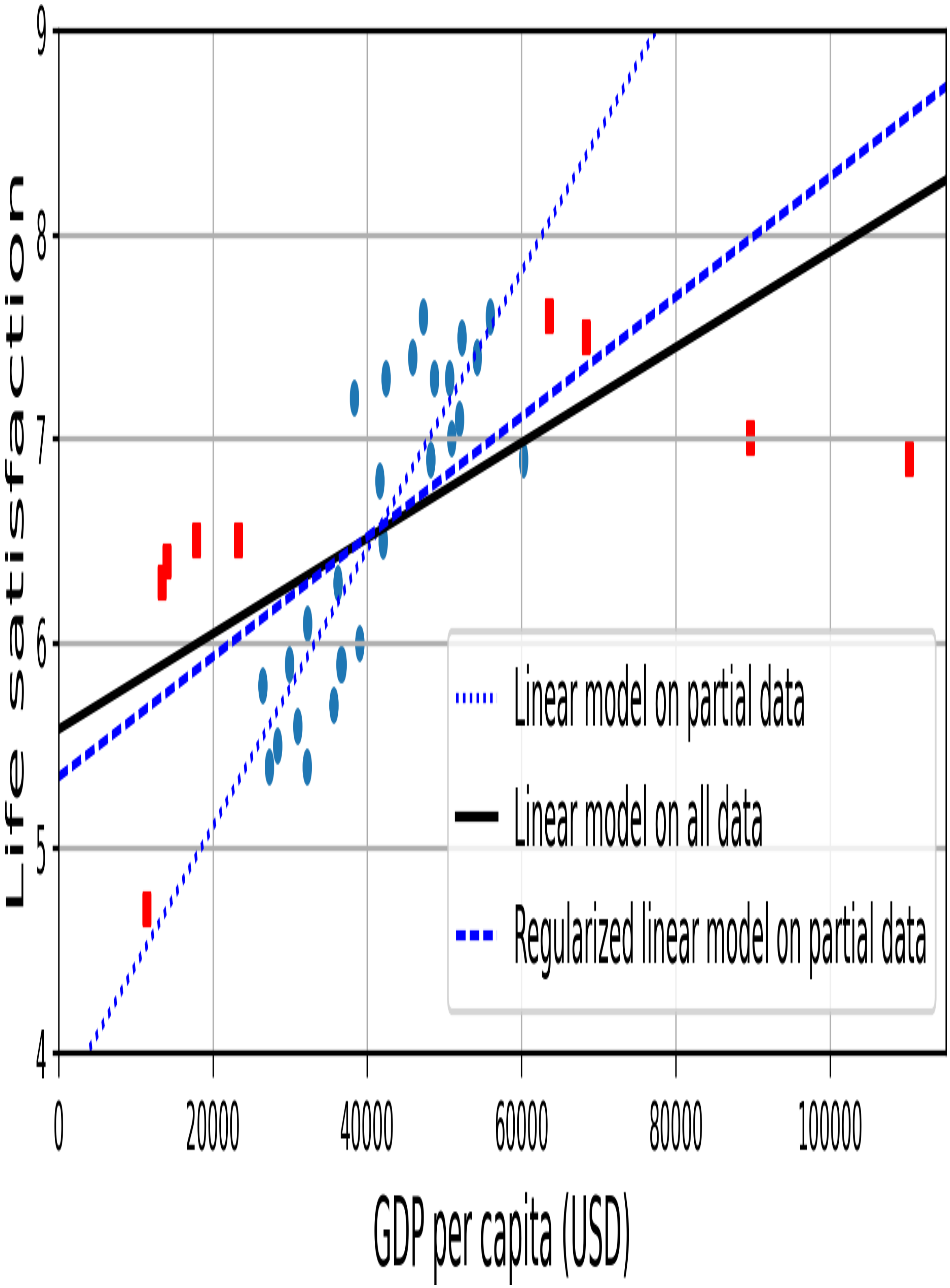


Figure 1-24. Regularization reduces the risk of overfitting

The amount of regularization to apply during learning can be controlled by a *hyperparameter*. A hyperparameter is a parameter of a learning algorithm (not of the model). As such, it is not affected by the learning algorithm itself; it must be set prior to training and remains constant during training. If you set the regularization hyperparameter to a very large value, you will get an almost flat model (a slope close to zero); the learning algorithm will almost certainly not overfit the training data, but it will be less likely to find a good solution. Tuning hyperparameters is an important part of building a Machine Learning system (you will see a detailed example in the next chapter).

Underfitting the Training Data

As you might guess, *underfitting* is the opposite of overfitting: it occurs when your model is too simple to learn the underlying structure of the data. For example, a linear model of life satisfaction is prone to underfit; reality is just more complex than the model, so its predictions are bound to be inaccurate, even on the training examples.

Here are the main options for fixing this problem:

- Select a more powerful model, with more parameters.
- Feed better features to the learning algorithm (feature engineering).
- Reduce the constraints on the model (e.g., reduce the regularization hyperparameter).

Stepping Back

By now you know a lot about Machine Learning. However, we went through so many concepts that you may be feeling a little lost, so let's step back and look at the big picture:

- Machine Learning is about making machines get better at some task by learning from data, instead of having to explicitly code rules.

- There are many different types of ML systems: supervised or not, batch or online, instance-based or model-based.
- In an ML project you gather data in a training set, and you feed the training set to a learning algorithm. If the algorithm is model-based, it tunes some parameters to fit the model to the training set (i.e., to make good predictions on the training set itself), and then hopefully it will be able to make good predictions on new cases as well. If the algorithm is instance-based, it just learns the examples by heart and generalizes to new instances by using a similarity measure to compare them to the learned instances.
- The system will not perform well if your training set is too small, or if the data is not representative, is noisy, or is polluted with irrelevant features (garbage in, garbage out). Lastly, your model needs to be neither too simple (in which case it will underfit) nor too complex (in which case it will overfit).

There's just one last important topic to cover: once you have trained a model, you don't want to just "hope" it generalizes to new cases. You want to evaluate it and fine-tune it if necessary. Let's see how to do that.

Testing and Validating

The only way to know how well a model will generalize to new cases is to actually try it out on new cases. One way to do that is to put your model in production and monitor how well it performs. This works well, but if your model is horribly bad, your users will complain—not the best idea.

A better option is to split your data into two sets: the *training set* and the *test set*. As these names imply, you train your model using the training set, and you test it using the test set. The error rate on new cases is called the *generalization error* (or *out-of-sample error*), and by evaluating your model on the test set, you get an estimate of this error. This value tells you how well your model will perform on instances it has never seen before.

If the training error is low (i.e., your model makes few mistakes on the training set) but the generalization error is high, it means that your model is overfitting the training data.

> **TIP**
>
> It is common to use 80% of the data for training and *hold out* 20% for testing. However, this depends on the size of the dataset: if it contains 10 million instances, then holding out 1% means your test set will contain 100,000 instances, probably more than enough to get a good estimate of the generalization error.

Hyperparameter Tuning and Model Selection

Evaluating a model is simple enough: just use a test set. But suppose you are hesitating between two types of models (say, a linear model and a polynomial model): how can you decide between them? One option is to train both and compare how well they generalize using the test set.

Now suppose that the linear model generalizes better, but you want to apply some regularization to avoid overfitting. The question is, how do you choose the value of the regularization hyperparameter? One option is to train 100 different models using 100 different values for this hyperparameter. Suppose you find the best hyperparameter value that produces a model with the lowest generalization error—say, just 5% error. You launch this model into production, but unfortunately it does not perform as well as expected and produces 15% errors. What just happened?

The problem is that you measured the generalization error multiple times on the test set, and you adapted the model and hyperparameters to produce the best model *for that particular set*. This means that the model is unlikely to perform as well on new data.

A common solution to this problem is called *holdout validation* (Figure 1-25): you simply hold out part of the training set to evaluate several candidate models and select the best one. The new held-out set is called the *validation set* (or the *development set*, or *dev set*). More specifically, you train multiple models with various hyperparameters on the reduced training set (i.e., the full training set minus the validation set), and you select the model that performs best on the validation set. After this holdout validation process, you train the best model on the full training set (including the validation set), and this gives you the final model. Lastly, you evaluate this final model on the test set to get an estimate of the generalization error.

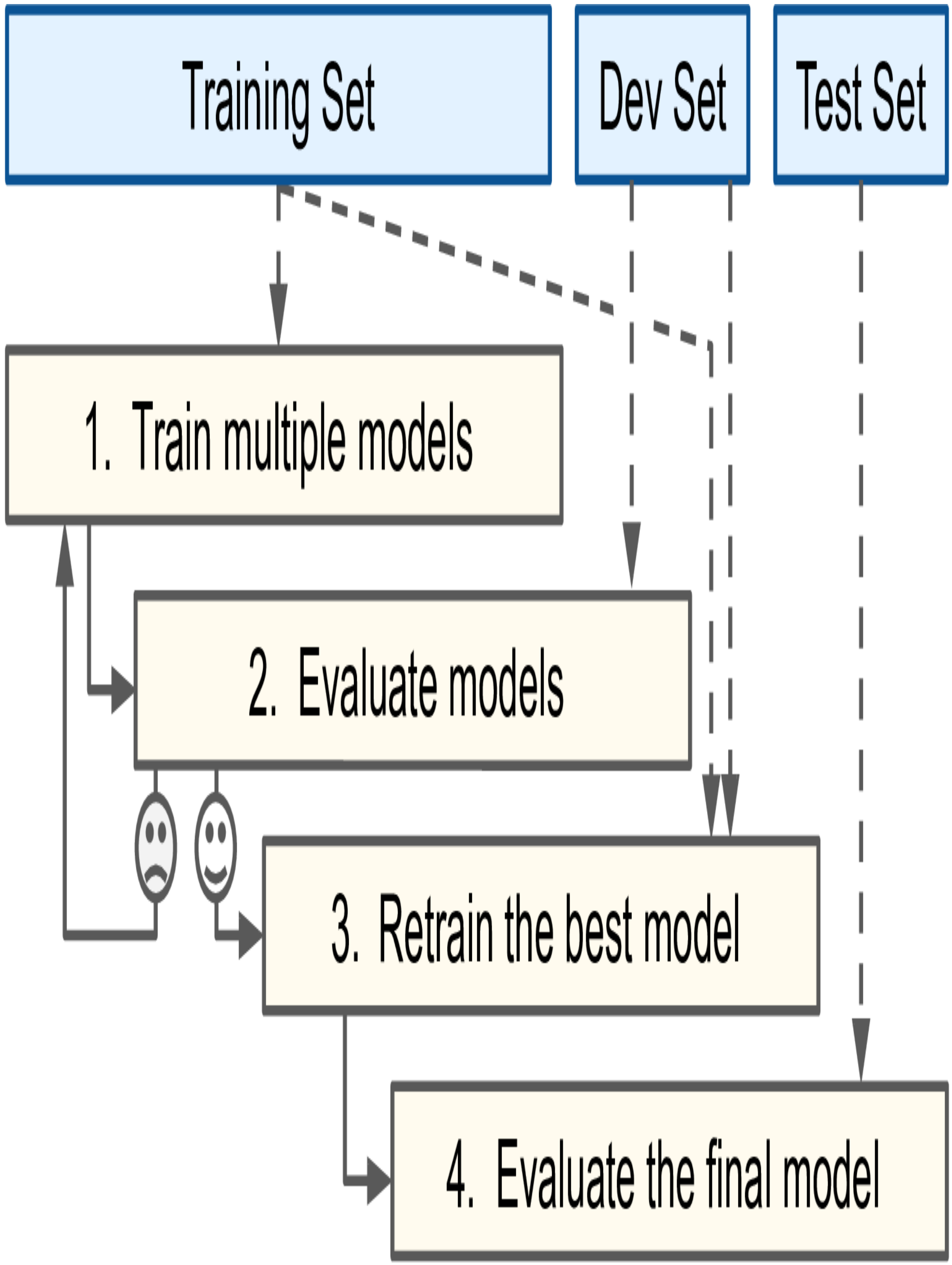


Figure 1-25. Model selection using holdout validation

This solution usually works quite well. However, if the validation set is too small, then model evaluations will be imprecise: you may end up selecting a suboptimal model by mistake. Conversely, if the validation set is too large, then the remaining training set will be much smaller than the full training set. Why is this bad? Well, since the final model will be trained on the full training set, it is not ideal to compare candidate models trained on a much smaller training set. It would be like selecting the fastest sprinter to participate in a marathon. One way to solve this problem is to perform repeated *cross-validation*, using many small validation sets. Each model is evaluated once per validation set after it is trained on the rest of the data. By averaging out all the evaluations of a model, you get a much more accurate measure of its performance. There is a drawback, however: the training time is multiplied by the number of validation sets.

Data Mismatch

In some cases, it's easy to get a large amount of data for training, but this data probably won't be perfectly representative of the data that will be used in production. For example, suppose you want to create a mobile app to take pictures of flowers and automatically determine their species. You can easily download millions of pictures of flowers on the web, but they won't be perfectly representative of the pictures that will actually be taken using the app on a mobile device. Perhaps you only have 1,000 representative pictures (i.e., actually taken with the app).

In this case, the most important rule to remember is that both the validation set and the test set must be as representative as possible of the data you expect to use in production, so they should be composed exclusively of representative pictures: you can shuffle them and put half in the validation set and half in the test set (making sure that no duplicates or near-duplicates end up in both sets). After training your model on the web pictures, if you observe that the performance of the model on the validation set is disappointing, you will not know whether this is because your model has overfit the training set, or whether this is just due to the mismatch between the web pictures and the mobile app pictures.

One solution is to hold out some of the training pictures (from the web) in yet another set that Andrew Ng dubbed the *train-dev set* (Figure 1-26). After the model is trained (on the training set, *not* on the train-dev set), you can evaluate it on the train-dev set. If the model performs poorly, then it must have overfit the training set, so you should try to simplify or regularize the model, get more training data, and clean up the training data. But if it performs well on the train-dev set, then you can evaluate the model on the dev set. If it performs poorly, then the problem must be coming from the data mismatch. You can try to tackle this problem by preprocessing the web images to make them look more like the pictures that will be taken by the mobile app, and then retraining the model. Once you have a model that performs well on both the train-dev set and the dev set, you can evaluate it one last time on the test set to know how well it is likely to perform in production.

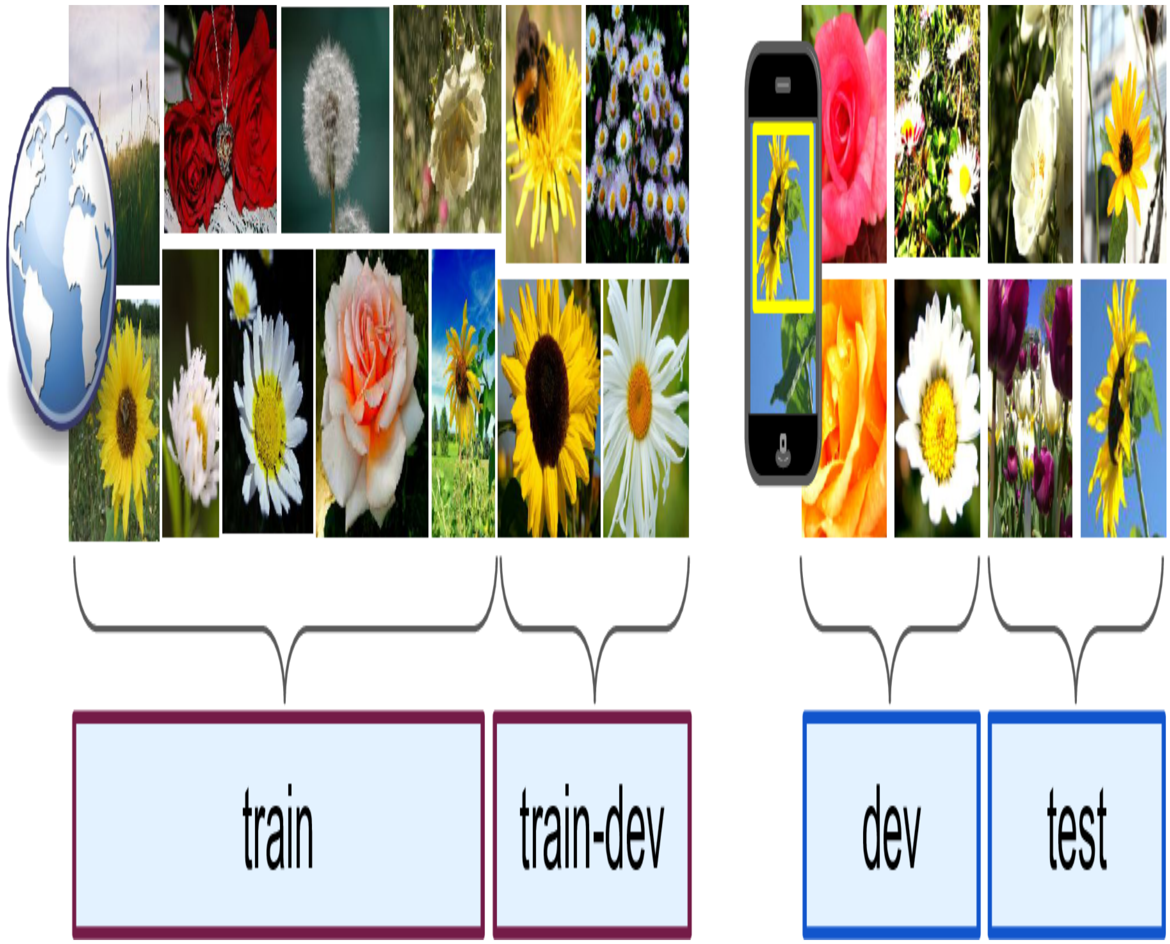


Figure 1-26. When real data is scarce (right), you may use similar abundant data (left) for training and hold out some of it in a train-dev set to evaluate overfitting. The real data is then used to evaluate data-mismatch (dev set), and to evaluate the final model's performance (test set).

NO FREE LUNCH THEOREM

A model is a simplified representation of the data. The simplifications are meant to discard the superfluous details that are unlikely to generalize to new instances. When you select a particular type of model, you are implicitly making *assumptions* about the data. For example, if you choose a linear model, you are implicitly assuming that the data is fundamentally linear and that the distance between the instances and the straight line is just noise, which can safely be ignored.

In a famous 1996 paper,[9] David Wolpert demonstrated that if you make absolutely no assumption about the data, then there is no reason to prefer one model over any other. This is called the *No Free Lunch* (NFL) theorem. For some datasets the best model is a linear model, while for other datasets it is a neural network. There is no model that is *a priori* guaranteed to work better (hence the name of the theorem). The only way to know for sure which model is best is to evaluate them all. Since this is not possible, in practice you make some reasonable assumptions about the data and evaluate only a few reasonable models. For example, for simple tasks you may evaluate linear models with various levels of regularization, and for a complex problem you may evaluate various neural networks.

Exercises

In this chapter we have covered some of the most important concepts in Machine Learning. In the next chapters we will dive deeper and write more code, but before we do, make sure you can answer the following questions:

1. How would you define Machine Learning?

2. Can you name four types of applications where it shines?

3. What is a labeled training set?

4. What are the two most common supervised tasks?
5. Can you name four common unsupervised tasks?
6. What type of algorithm would you use to allow a robot to walk in various unknown terrains?
7. What type of algorithm would you use to segment your customers into multiple groups?
8. Would you frame the problem of spam detection as a supervised learning problem or an unsupervised learning problem?
9. What is an online learning system?
10. What is out-of-core learning?
11. What type of algorithm relies on a similarity measure to make predictions?
12. What is the difference between a model parameter and a model hyperparameter?
13. What do model-based algorithms search for? What is the most common strategy they use to succeed? How do they make predictions?
14. Can you name four of the main challenges in Machine Learning?
15. If your model performs great on the training data but generalizes poorly to new instances, what is happening? Can you name three possible solutions?
16. What is a test set, and why would you want to use it?
17. What is the purpose of a validation set?
18. What is the train-dev set, when do you need it, and how do you use it?
19. What can go wrong if you tune hyperparameters using the test set?

Solutions to these exercises are available at the end of this chapter's notebook, at *https://homl.info/colab3*.

---

1 Fun fact: this odd-sounding name is a statistics term introduced by Francis Galton while he was studying the fact that the children of tall people tend to be shorter than their parents. Since the children were shorter, he called this *regression to the mean*. This name was then applied to the methods he used to analyze correlations between variables.

2 Notice how animals are rather well separated from vehicles and how horses are close to deer but far from birds. Figure reproduced with permission from Richard Socher et al., "Zero-Shot Learning Through Cross-Modal Transfer," *Proceedings of the 26th International Conference on Neural Information Processing Systems* 1 (2013): 935–943.

3 That's when the system works perfectly. In practice it often creates a few clusters per person, and sometimes mixes up two people who look alike, so you may need to provide a few labels per person and manually clean up some clusters.

4 By convention, the Greek letter θ (theta) is frequently used to represent model parameters.

5 It's OK if you don't understand all the code yet; I will present Scikit-Learn in the following chapters.

6 For example, knowing whether to write "to," "two," or "too," depending on the context.

7 Figure reproduced with permission from Michele Banko and Eric Brill, "Scaling to Very Very Large Corpora for Natural Language Disambiguation," *Proceedings of the 39th Annual Meeting of the Association for Computational Linguistics* (2001): 26–33.

8 Peter Norvig et al., "The Unreasonable Effectiveness of Data," *IEEE Intelligent Systems* 24, no. 2 (2009): 8–12.

9 David Wolpert, "The Lack of A Priori Distinctions Between Learning Algorithms," *Neural Computation* 8, no. 7 (1996): 1341–1390.

Chapter 2. End-to-End Machine Learning Project

A NOTE FOR EARLY RELEASE READERS

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.

This will be the 2nd chapter of the final book. Notebooks are available on GitHub at *https://github.com/ageron/handson-ml3*. Datasets are available at *https://github.com/ageron/data*.

If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the editoor at ntache@oreilly.com.

In this chapter you will work through an example project end to end, pretending to be a recently hired data scientist at a real estate company. The example project is fictitious; the goal is to illustrate the main steps of a Machine Learning project, not to learn anything about the real estate business. Here are the main steps we will walk through:

1. Look at the big picture.
2. Get the data.
3. Explore and visualize the data to gain insights.
4. Prepare the data for Machine Learning algorithms.
5. Select a model and train it.
6. Fine-tune your model.
7. Present your solution.

8. Launch, monitor, and maintain your system.

Working with Real Data

When you are learning about Machine Learning, it is best to experiment with real-world data, not artificial datasets. Fortunately, there are thousands of open datasets to choose from, ranging across all sorts of domains. Here are a few places you can look to get data:

- Popular open data repositories
  - OpenML.org
  - Kaggle.com
  - PapersWithCode.com
  - UC Irvine Machine Learning Repository
  - Amazon's AWS datasets
  - TensorFlow Datasets
- Meta portals (they list open data repositories)
  - DataPortals.org
  - OpenDataMonitor.eu
- Other pages listing many popular open data repositories
  - Wikipedia's list of Machine Learning datasets
  - Quora.com
  - The datasets subreddit

In this chapter we'll use the California Housing Prices dataset from the StatLib repository[1] (see Figure 2-1). This dataset is based on data from the 1990 California census. It is not exactly recent (a nice house in the Bay Area was still affordable at the time), but it has many qualities for learning, so we will pretend it is recent data. For teaching purposes I’ve added a categorical attribute and removed a few features.

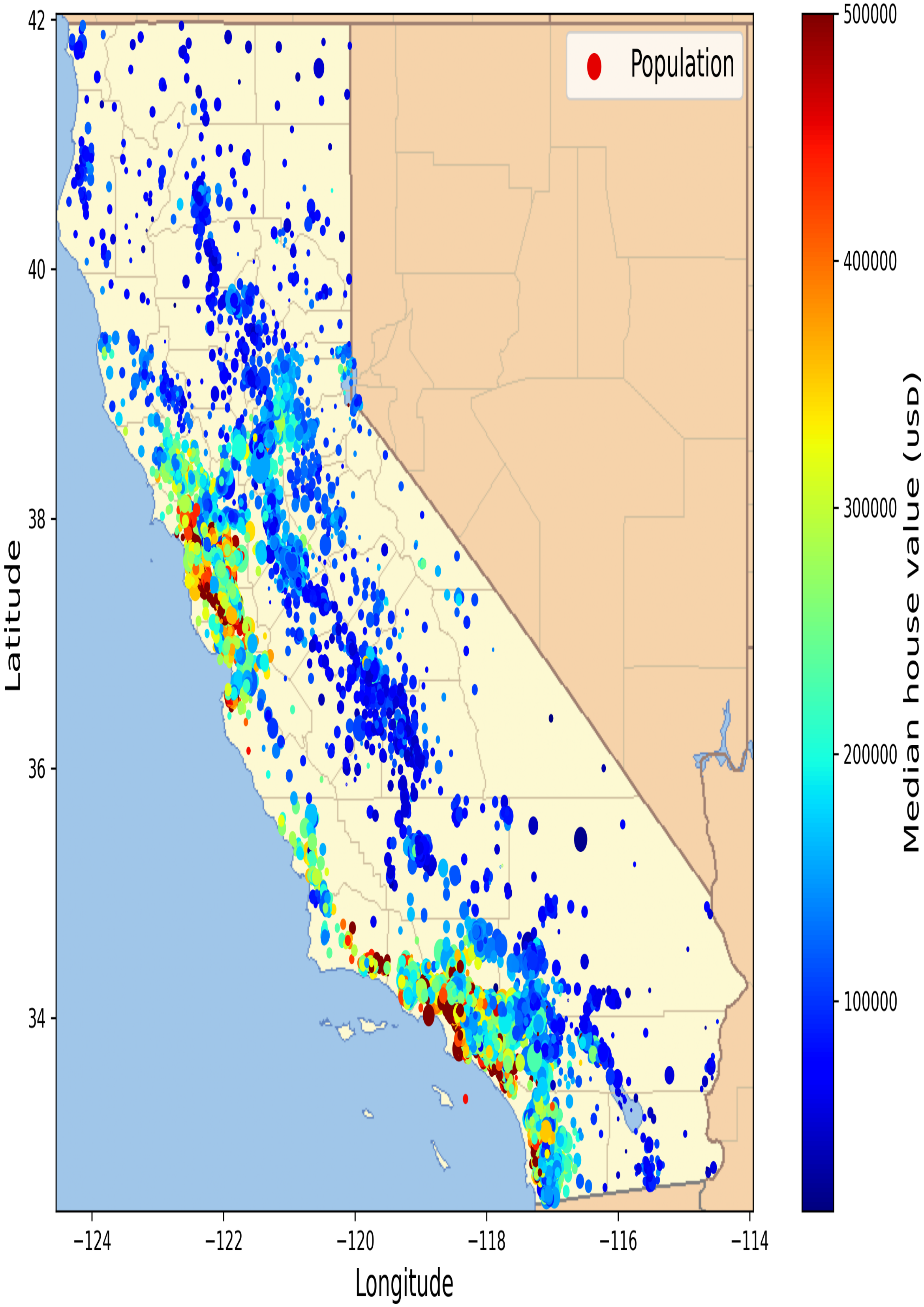


Figure 2-1. California housing prices

Look at the Big Picture

Welcome to the Machine Learning Housing Corporation! Your first task is to use California census data to build a model of housing prices in the state. This data includes metrics such as the population, median income, and median housing price for each block group in California. Block groups are the smallest geographical unit for which the US Census Bureau publishes sample data (a block group typically has a population of 600 to 3,000 people). I will call them "districts" for short.

Your model should learn from this data and be able to predict the median housing price in any district, given all the other metrics.

> **TIP**
>
> Since you are a well-organized data scientist, the first thing you should do is pull out your Machine Learning project checklist. You can start with the one in Appendix A; it should work reasonably well for most Machine Learning projects, but make sure to adapt it to your needs. In this chapter we will go through many checklist items, but we will also skip a few, either because they are self-explanatory or because they will be discussed in later chapters.

Frame the Problem

The first question to ask your boss is what exactly the business objective is. Building a model is probably not the end goal. How does the company expect to use and benefit from this model? Knowing the objective is important because it will determine how you frame the problem, which algorithms you will select, which performance measure you will use to evaluate your model, and how much effort you will spend tweaking it.

Your boss answers that your model's output (a prediction of a district's median housing price) will be fed to another Machine Learning system (see Figure 2-2), along with many other signals.[2] This downstream system will determine whether it is worth investing in a given area or not. Getting this right is critical, as it directly affects revenue.

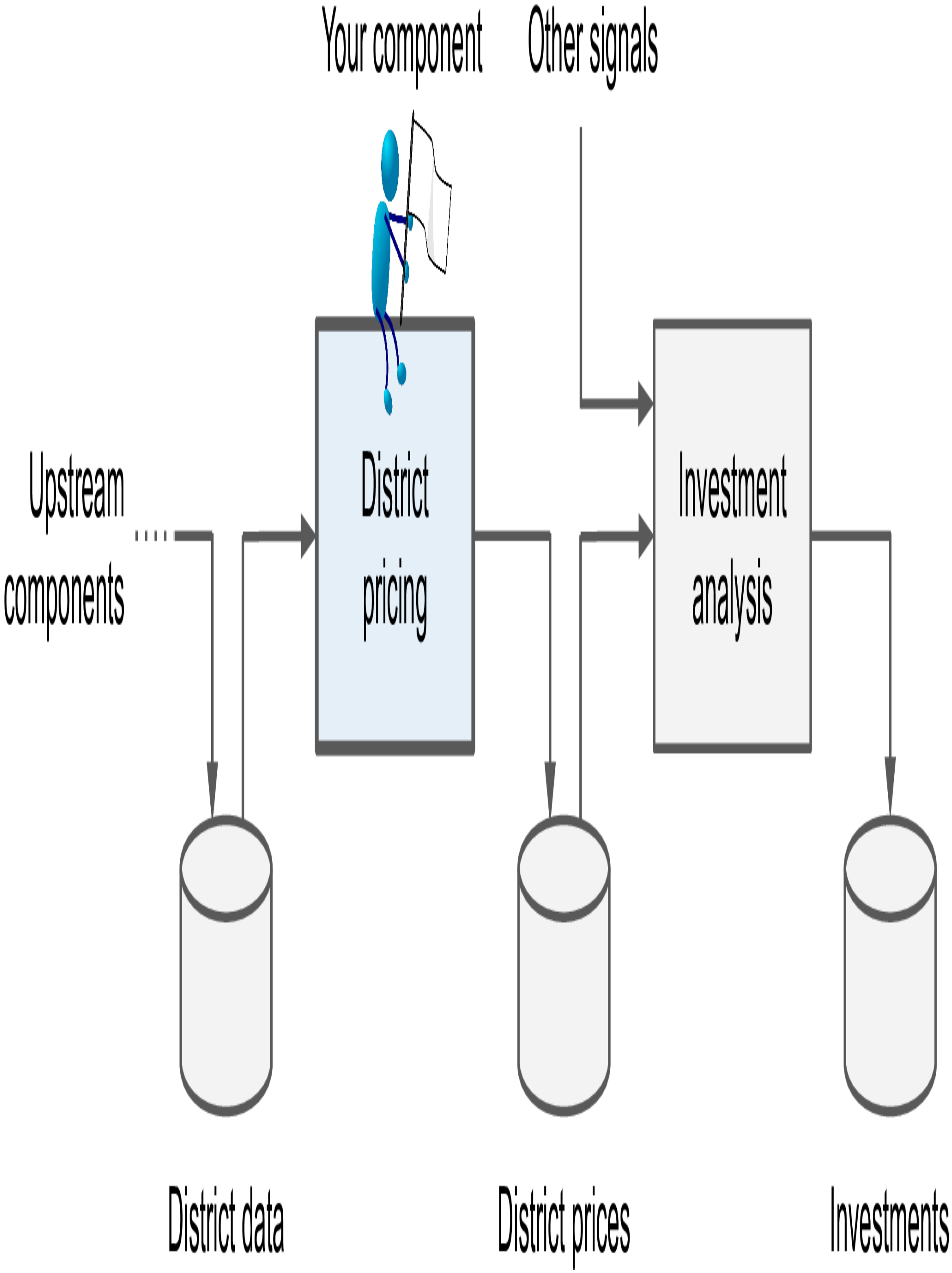


Figure 2-2. A Machine Learning pipeline for real estate investments

PIPELINES

A sequence of data processing components is called a data *pipeline*. Pipelines are very common in Machine Learning systems, since there is a lot of data to manipulate and many data transformations to apply.

Components typically run asynchronously. Each component pulls in a large amount of data, processes it, and spits out the result in another data store. Then, some time later, the next component in the pipeline pulls this data and spits out its own output. Each component is fairly self-contained: the interface between components is simply the data store. This makes the system simple to grasp (with the help of a data flow graph), and different teams can focus on different components. Moreover, if a component breaks down, the downstream components can often continue to run normally (at least for a while) by just using the last output from the broken component. This makes the architecture quite robust.

On the other hand, a broken component can go unnoticed for some time if proper monitoring is not implemented. The data gets stale and the overall system's performance drops.

The next question to ask your boss is what the current solution looks like (if any). The current situation will often give you a reference for performance, as well as insights on how to solve the problem. Your boss answers that the district housing prices are currently estimated manually by experts: a team gathers up-to-date information about a district, and when they cannot get the median housing price, they estimate it using complex rules.

This is costly and time-consuming, and their estimates are not great; in cases where they manage to find out the actual median housing price, they often realize that their estimates were off by more than 30%. This is why the company thinks that it would be useful to train a model to predict a district's median housing price, given other data about that district. The census data looks like a great dataset to exploit for this purpose, since it includes the median housing prices of thousands of districts, as well as other data.

With all this information, you are now ready to start designing your system. First, determine what kind of training supervision the model will need: is it supervised, unsupervised, semi-supervised, self-supervised, or Reinforcement Learning? And is it a classification task, a regression task, or something else? Should you use batch learning or online learning techniques? Before you read on, pause and try to answer these questions for yourself.

Have you found the answers? Let's see: it is clearly a typical supervised learning task, since the model can be trained with *labeled* examples (each instance comes with the expected output, i.e., the district's median housing price). It is also a typical regression task, since the model will be asked to predict a value. More specifically, this is a *multiple regression* problem, since the system will use multiple features to make a prediction (it will use the district's population, the median income, etc.). It is also a *univariate regression* problem, since we are only trying to predict a single value for each district. If we were trying to predict multiple values per district, it would be a *multivariate regression* problem. Finally, there is no continuous flow of data coming into the system, there is no particular need to adjust to changing data rapidly, and the data is small enough to fit in memory, so plain batch learning should do just fine.

> **TIP**
>
> If the data were huge, you could either split your batch learning work across multiple servers (using the MapReduce technique) or use an online learning technique.

Select a Performance Measure

Your next step is to select a performance measure. A typical performance measure for regression problems is the Root Mean Square Error (RMSE). It gives an idea of how much error the system typically makes in its predictions, with a higher weight given to large errors. Equation 2-1 shows the mathematical formula to compute the RMSE.

Equation 2-1. Root Mean Square Error (RMSE)

$$\mathrm{RMSE}\left(\mathbf{X}, h\right) = \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(h\left(\mathbf{x}^{(i)}\right) - y^{(i)}\right)^2}$$

NOTATIONS

This equation introduces several very common Machine Learning notations that I will use throughout this book:

- m is the number of instances in the dataset you are measuring the RMSE on.
    - For example, if you are evaluating the RMSE on a validation set of 2,000 districts, then m = 2,000.
- $\mathbf{x}^{(i)}$ is a vector of all the feature values (excluding the label) of the i^{th} instance in the dataset, and $y^{(i)}$ is its label (the desired output value for that instance).
    - For example, if the first district in the dataset is located at longitude –118.29°, latitude 33.91°, and it has 1,416 inhabitants with a median income of $38,372, and the median house value is $156,400 (ignoring the other features for now), then:

$$\mathbf{x}^{(1)} = \begin{pmatrix} -118.29 \\ 33.91 \\ 1{,}416 \\ 38{,}372 \end{pmatrix}$$

      and:

$$y^{(1)} = 156{,}400$$

- $\mathbf{X}$ is a matrix containing all the feature values (excluding labels) of all instances in the dataset. There is one row per instance, and the i^{th} row is equal to the transpose of $\mathbf{x}^{(i)}$, noted $(\mathbf{x}^{(i)})^{\intercal}$.[3]
    - For example, if the first district is as just described, then the matrix $\mathbf{X}$ looks like this:

$$\mathbf{X} = \begin{pmatrix} \left(\mathbf{x}^{(1)}\right)^\top \\ \left(\mathbf{x}^{(2)}\right)^\top \\ \vdots \\ \left(\mathbf{x}^{(1999)}\right)^\top \\ \left(\mathbf{x}^{(2000)}\right)^\top \end{pmatrix} = \begin{pmatrix} -118.29 & 33.91 & 1{,}416 & 38{,}372 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

- h is your system's prediction function, also called a *hypothesis*. When your system is given an instance's feature vector $\mathbf{x}^{(i)}$, it outputs a predicted value $\hat{y}^{(i)} = h(\mathbf{x}^{(i)})$ for that instance ($\hat{y}$ is pronounced "y-hat").
    - For example, if your system predicts that the median housing price in the first district is \$158,400, then $\hat{y}^{(1)} = h(\mathbf{x}^{(1)}) = 158{,}400$. The prediction error for this district is $\hat{y}^{(1)} - y^{(1)} = 2{,}000$.
- RMSE($\mathbf{X}$,h) is the cost function measured on the set of examples using your hypothesis h.

We use lowercase italic font for scalar values (such as m or $y^{(i)}$) and function names (such as h), lowercase bold font for vectors (such as $\mathbf{x}^{(i)}$), and uppercase bold font for matrices (such as $\mathbf{X}$).

Even though the RMSE is generally the preferred performance measure for regression tasks, in some contexts you may prefer to use another function. For example, suppose that there are many outlier districts. In that case, you may consider using the *mean absolute error* (MAE, also called the average absolute deviation; see Equation 2-2):

Equation 2-2. Mean absolute error (MAE)

$$\mathrm{MAE}\left(\mathbf{X}, h\right) = \frac{1}{m}\sum_{i=1}^{m}\left|h\left(\mathbf{x}^{(i)}\right) - y^{(i)}\right|$$

Both the RMSE and the MAE are ways to measure the distance between two vectors: the vector of predictions and the vector of target values. Various distance measures, or *norms*, are possible:

- Computing the root of a sum of squares (RMSE) corresponds to the *Euclidean norm*: this is the notion of distance you are familiar with. It is also called the ℓ_2 *norm*, noted $\| \cdot \|_2$ (or just $\| \cdot \|$).
- Computing the sum of absolutes (MAE) corresponds to the ℓ_1 *norm*, noted $\| \cdot \|_1$. This is sometimes called the *Manhattan norm* because it measures the distance between two points in a city if you can only travel along orthogonal city blocks.
- More generally, the ℓ_k *norm* of a vector $\mathbf{v}$ containing n elements is defined as $\|\mathbf{v}\|_k = (|v_0|^k + |v_1|^k + ... + |v_n|^k)^{1/k}$. ℓ_0 gives the number of nonzero elements in the vector, and ℓ_∞ gives the maximum absolute value in the vector.
- The higher the norm index, the more it focuses on large values and neglects small ones. This is why the RMSE is more sensitive to outliers than the MAE. But when outliers are exponentially rare (like in a bell-shaped curve), the RMSE performs very well and is generally preferred.

Check the Assumptions

Lastly, it is good practice to list and verify the assumptions that have been made so far (by you or others); this can help you catch serious issues early on. For example, the district prices that your system outputs are going to be fed into a downstream Machine Learning system, and you assume that these prices are going to be used as such. But what if the downstream system converts the prices into categories (e.g., “cheap,” “medium,” or “expensive”) and then uses those categories instead of the prices themselves? In this case, getting the price perfectly right is not important at all; your system just needs to get the category right. If that’s so, then the problem should have been framed as a classification task, not a regression task. You don’t want to find this out after working on a regression system for months.

Fortunately, after talking with the team in charge of the downstream system, you are confident that they do indeed need the actual prices, not just categories. Great! You’re all set, the lights are green, and you can start coding now!

Get the Data

It’s time to get your hands dirty. Don’t hesitate to pick up your laptop and walk through the code examples. As I mentioned in the preface, all the code examples in this book are open source and available online at *https://github.com/ageron/handson-ml3*, as Jupyter notebooks, which are interactive documents containing text, images, and executable code snippets (Python in our case). In this book I will assume you are running these notebooks on Google Colab, a free service that lets you run any Jupyter notebook directly online, without having to install anything on your machine. But if you want to use another online platform (e.g., Kaggle kernels) or if you want to install everything locally on your own machine, please see the instructions on this project’s home page at the GitHub page (above).

Running the Code Examples Using Google Colab

First, open a web browser and visit *https://homl.info/colab3*: this will lead you to Google Colab, and it will display the list of Jupyter notebooks for this book (see Figure 2-3). You will find one notebook per chapter, plus a few extra notebooks, including an extra chapter on Support Vector Machines, and tutorials for NumPy, Matplotlib, Pandas, Linear Algebra and Differential Calculus.

Figure 2-3. List of notebooks in Google Colab

For example, if you click on `02_end_to_end_machine_learning_project.ipynb`, the notebook from Chapter 2 will open up in Google Colab (see Figure 2-4).

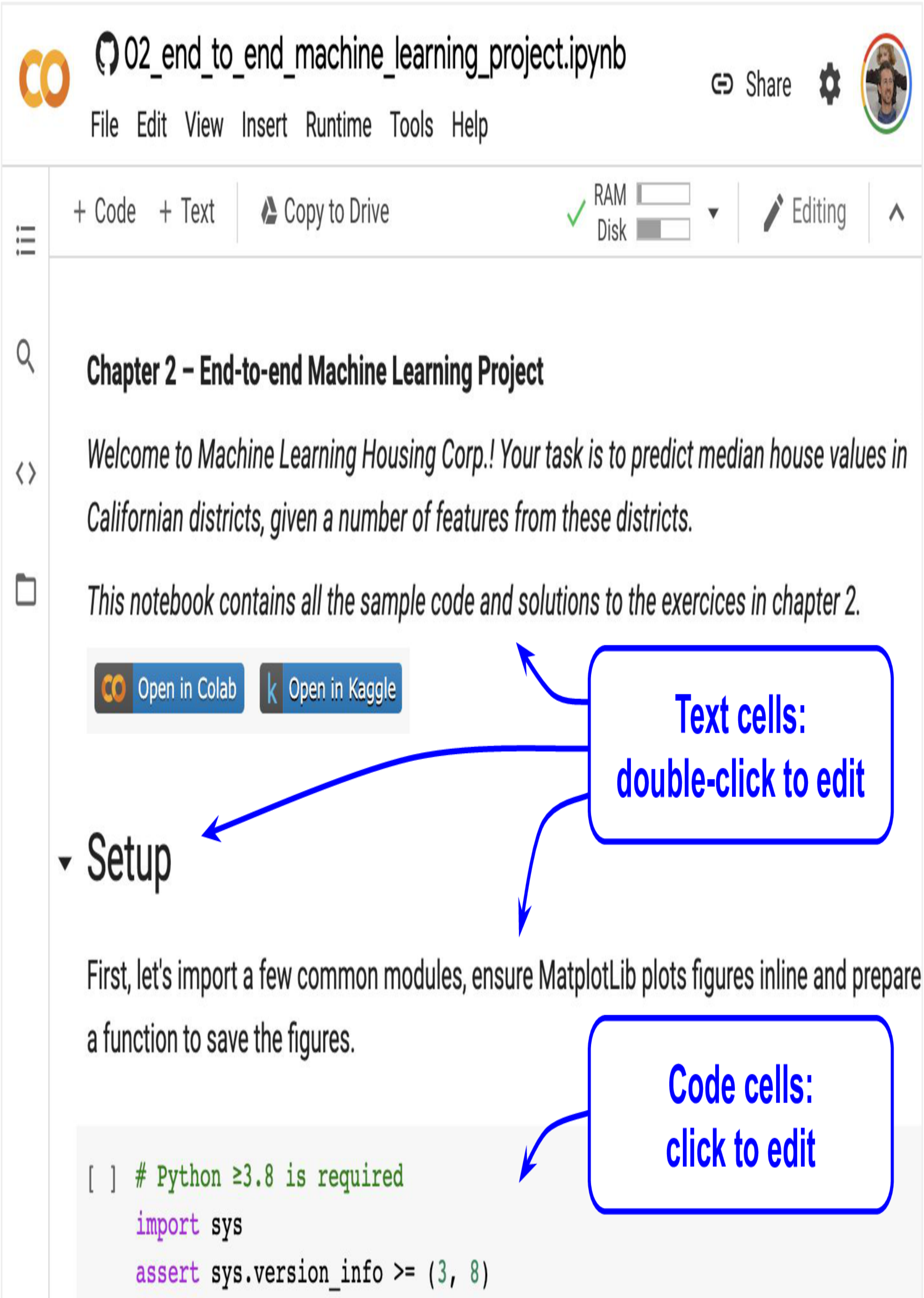


Figure 2-4. Your notebook in Google Colab

A Jupyter notebook is composed of a list of cells. Each cell contains either executable code or text. Try double-clicking on the first text cell (which contains the sentence “Welcome to Machine Learning Housing Corp.!”). This will open the cell for editing. Notice that Jupyter notebooks use Markdown syntax for formatting (e.g., `**bold**`, `*italics*`, `# Title`, `[url](link text)`, and so on). Try modifying this text, then press **Shift-Enter** to see the result.

Next, create a new code cell by selecting Insert > Code cell from the menu. Alternatively, you can click the `+ Code` button in the toolbar, or hover your mouse over the bottom of a cell until you see `+ Code` and `+ Text` appear, then click on `+ Code`. In the new code cell, type some Python code, such as `print("Hello World")` then press **Shift-Enter** to run this code (or click on the ▷ button on the left side of the cell).

If you are not logged in to your Google Account, you will be asked to login now (if you don’t already have a Google account, you will need to create one). Once you are logged in and you try to run the code, you will get a security warning telling you that this notebook was not authored by Google. Indeed, a malicious person could create a notebook that tries to trick you into entering your Google credentials so they can access your personal data. So before you run a notebook, always make sure you trust its author (or double-check what each code cell will do before running it). Now, assuming you trust me (or you plan to check every code cell), you can go ahead and click “Run anyway”.

Colab will then allocate a new *Runtime* for you: this is a free virtual machine located on Google’s servers, containing a bunch of tools and Python libraries, including everything we need for most chapters (in some chapters, we will need to run a command to install some additional libraries). This will take a few seconds. Next, Colab will automatically connect to this Runtime and use it to execute your new code cell. Importantly, the code runs on the Runtime, *not* on your machine. The code’s output will be displayed under the cell. Congrats, you’ve run some Python code on Colab!

TIP

To insert a new code cell, you can also type **Ctrl-m** (or **Cmd-m** on macOS) followed by **a** (to insert **a**bove the active cell) or **b** (to insert **b**elow). There are many other keyboard shortcuts available: you can view and edit them by typing **Ctrl-m** (or **Cmd-m**) then **h**. If you choose to run the notebooks on Kaggle or on your own machine using JupyterLab or an IDE such as Visual Studio Code with the Jupyter extension, you will see some minor differences: Runtimes are called *Kernels*, the User Interface and keyboard shortcuts are slightly different, etc. But switching from one Jupyter environment to another is not too hard.

Saving Your Code Changes and Your Data

You can make changes to a Colab notebook, and they will persist for as long as you keep your browser tab open, but once you close it, the changes will be lost. To avoid this, make sure you save a copy of the notebook to your Google Drive by selecting File > Save a copy in Drive. Alternatively, you can download the notebook to your computer by selecting File > Download > Download .ipynb. Either way, you can later visit *https://colab.research.google.com/* and open the notebook again (either from Google Drive or by uploading it from your computer).

WARNING

Google Colab is meant only for interactive use: you can play around in the notebooks and tweak the code as you like, but you cannot let the notebooks run unattended for a long period of time, or else the Runtime will be shutdown and all of its data will be lost.

If the notebook generates data that you care about, make sure you download this data before the Runtime shuts down. To do this, click on the Files icon (see step 1 in Figure 2-5), find the file you want to download, click on the vertical dots next to it (step 2), and click Download (step 3).

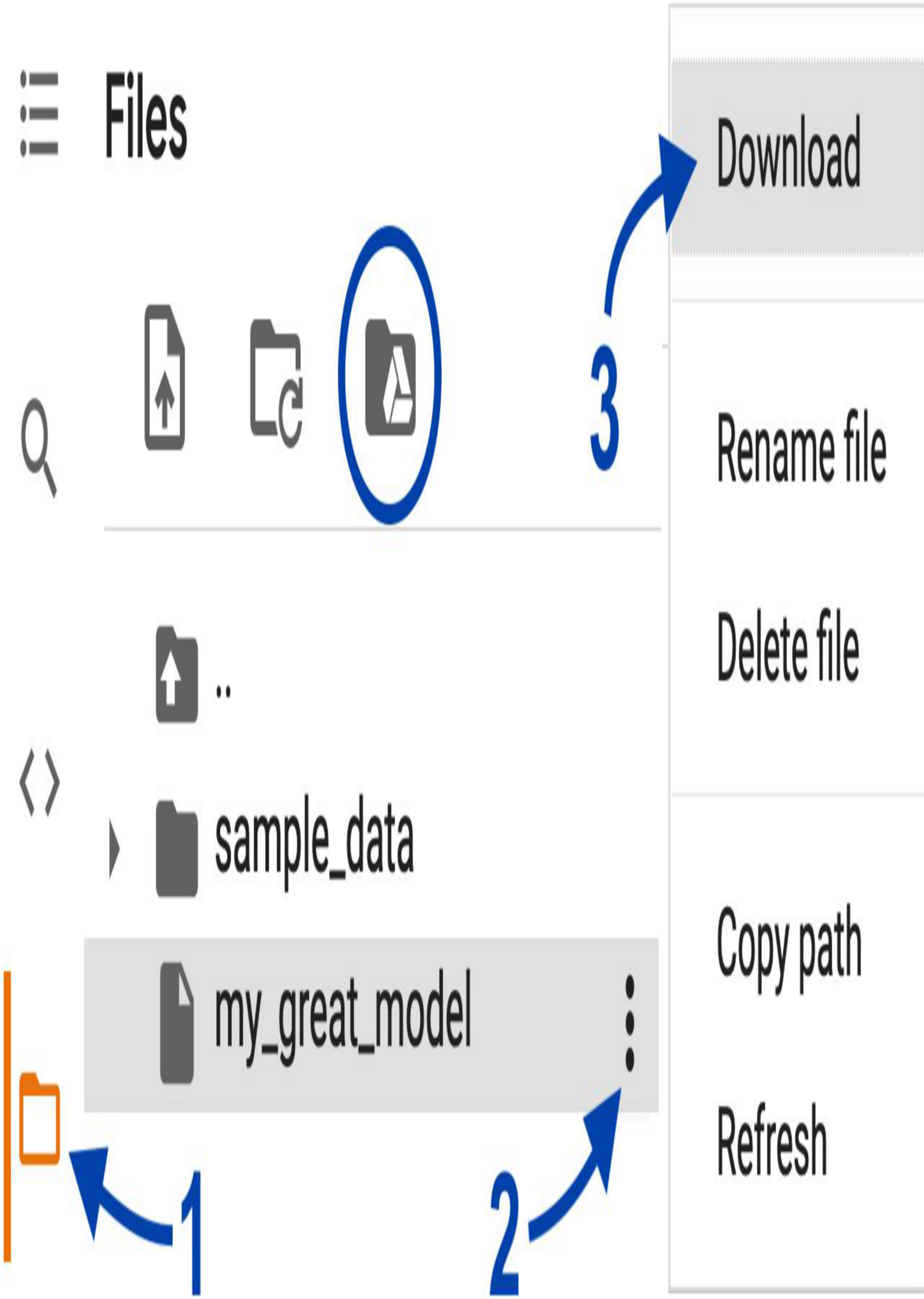

Files
..
sample_data
my_great_model
Download
Rename file
Delete file
Copy path
Refresh
1
2
3

Figure 2-5. Downloading a file from a Google Colab Runtime (steps 1 to 3), or mounting your Google Drive (circled icon)

Alternatively, you can mount your Google Drive on the Runtime, allowing the notebook to read and write files directly to Google Drive, as if it were a local directory. For this, click on the Files icon (step 1) then click on the Google Drive icon (circled in Figure 2-5) and follow the on-screen instructions. By default, your Google Drive will be mounted at `/content/drive/MyDrive`. If you want to backup a data file, simply copy it to this directory by running `!cp /content/my_great_model /content/drive/MyDrive`. Any command starting with a bang (`!`) is treated as a shell command, not as Python code: `cp` is the Linux shell command to copy a file from one path to another. Note that Colab Runtimes run on Linux (specifically, Ubuntu).

The Power and Danger of Interactivity

Jupyter notebooks are interactive, and that's a great thing: you can run each cell one by one, stop at any point, insert a cell, play with the code, go back and run the same cell again, etc., and I highly encourage you to do so. If you just run the cells one by one without ever playing with them, you won't learn as fast. However, this flexibility comes at a price: it's very easy to run cells in the wrong order, or to forget to run a cell. If this happens, the subsequent code cells are likely to fail. For example, the very first code cell in each notebook contains setup code (such as imports), so make sure you run it first, or else nothing will work.

> **TIP**
>
> If you ever run into a weird error, try restarting the Runtime (by selecting Runtime > Restart runtime from the menu) and then run all the cells again from the beginning of the notebook: this will often solve the problem. If not, then it's likely that one of the changes you made broke the notebook: just revert to the original notebook and try again. If it still fails, then please file an issue on GitHub.

Book Code vs Notebook Code

You may sometimes notice some little differences between the code in this book and the code in the notebooks. This may happen for several reasons:

- A library may have changed slightly by the time you read these lines, or perhaps despite my best efforts I made an error in the book. Sadly, I cannot magically fix the code in your copy of this book (unless you are reading an electronic copy and you can download the latest version), but I *can* fix the notebooks: so if you run into an error after copying code from this book, please look for the fixed code in the notebooks: I will strive to keep them error-free and up-to-date with the latest library versions.
- The notebooks contain some extra code to beautify the figures (adding labels, setting font size, etc.), and to save them in high resolution for this book. You can safely ignore this extra code if you want.

I optimized the code for readability and simplicity: I made it as linear and flat as possible, defining very few functions or classes. The goal is to ensure that the code you are running is generally right in front of you, and not nested within several layers of abstractions that you have to search through. This also makes it easier for you to play with the code. For simplicity, there's limited error handling, and I placed some of the least common imports right where they are needed (instead of placing them at the top of the file, as is recommended by the PEP 8 Python style guide). That said, your production code will not be very different: just a bit more modular, and with additional tests and error handling, that's all.

OK! Once you're comfortable with Colab, you're ready to download the data.

Download the Data

In typical environments your data would be available in a relational database or some other common data store, and spread across multiple tables/documents/files. To access it, you would first need to get your credentials and access authorizations[4] and familiarize yourself with the data schema. In this project, however, things are much simpler: you will just download a single compressed file, *housing.tgz*, which contains a comma-separated values (CSV) file called *housing.csv* with all the data.

Rather than manually downloading and decompressing the data, it's usually preferable to write a function that does it for you. This is useful in particular if the data changes regularly: you can write a small script that uses the function to fetch the latest data (or you can set up a scheduled job to do that automatically at regular intervals). Automating the process of fetching the data is also useful if you need to install the dataset on multiple machines.

Here is the function to fetch and load the data:

```
from pathlib import Path
import pandas as pd
import tarfile
import urllib.request

def load_housing_data():
    tarball_path = Path("datasets/housing.tgz")
    if not tarball_path.is_file():
        Path("datasets").mkdir(parents=True, exist_ok=True)
        url = "https://github.com/ageron/data/raw/main/housing.tgz"
        urllib.request.urlretrieve(url, tarball_path)
        with tarfile.open(tarball_path) as housing_tarball:
            housing_tarball.extractall(path="datasets")
    return pd.read_csv(Path("datasets/housing/housing.csv"))

housing = load_housing_data()
```

When `load_housing_data()` is called, it looks for the *datasets/housing.tgz* file, and if it does not find it, it creates the *datasets* directory inside the current directory (which is */content* by default, in Colab), it downloads the *housing.tgz* file from the *ageron/data* GitHub repository, it extracts its content into the *datasets* directory, and this creates the *datasets*/*housing* directory with the *housing.csv* file inside it. Lastly, the function loads this CSV file into a Pandas DataFrame object containing all the data, and it returns it.

Take a Quick Look at the Data Structure

Let's take a look at the top five rows of data using the DataFrame's `head()` method (see Figure 2-6).

```
housing.head()
```

	longitude	latitude	housing_median_age	median_income	ocean_proximity	median_house_value
0	-122.23	37.88	41.0	8.3252	NEAR BAY	452600.0
1	-122.22	37.86	21.0	8.3014	NEAR BAY	358500.0
2	-122.24	37.85	52.0	7.2574	NEAR BAY	352100.0
3	-122.25	37.85	52.0	5.6431	NEAR BAY	341300.0
4	-122.25	37.85	52.0	3.8462	NEAR BAY	342200.0

Figure 2-6. Top five rows in the dataset

Each row represents one district. There are 10 attributes (they are not all shown in the screenshot): `longitude`, `latitude`, `housing_median_age`, `total_rooms`, `total_bedrooms`, `population`, `households`, `median_income`, `median_house_value`, and `ocean_proximity`.

The `info()` method is useful to get a quick description of the data, in particular the total number of rows, each attribute's type, and the number of non-null values:

```
>>> housing.info()
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 20640 entries, 0 to 20639
Data columns (total 10 columns):
 #   Column              Non-Null Count  Dtype
---  ------              --------------  -----
 0   longitude           20640 non-null  float64
 1   latitude            20640 non-null  float64
 2   housing_median_age  20640 non-null  float64
 3   total_rooms         20640 non-null  float64
 4   total_bedrooms      20433 non-null  float64
 5   population          20640 non-null  float64
 6   households          20640 non-null  float64
 7   median_income       20640 non-null  float64
 8   median_house_value  20640 non-null  float64
 9   ocean_proximity     20640 non-null  object
dtypes: float64(9), object(1)
memory usage: 1.6+ MB
```

NOTE

In this book, when a code example contains a mix of code and outputs, as is the case here, it is formatted like in the Python interpreter, for better readability: the code lines are prefixed with >>> (or `...` for indented blocks), and the outputs have no prefix.

There are 20,640 instances in the dataset, which means that it is fairly small by Machine Learning standards, but it's perfect to get started. Notice that the `total_bedrooms` attribute has only 20,433 non-null values, meaning that 207 districts are missing this feature. We will need to take care of this later.

All attributes are numerical, except the `ocean_proximity` field. Its type is `object`, so it could hold any kind of Python object. But since you loaded this data from a CSV file, you know that it must be a text attribute. When you looked at the top five rows, you probably noticed that the values in the ocean_proximity column were repetitive, which means that it is probably a categorical attribute. You can find out what categories exist and how many districts belong to each category by using the value_counts() method:

```
>>> housing["ocean_proximity"].value_counts()
<1H OCEAN     9136
INLAND        6551
NEAR OCEAN    2658
NEAR BAY      2290
ISLAND           5
Name: ocean_proximity, dtype: int64
```

Let’s look at the other fields. The describe() method shows a summary of the numerical attributes (Figure 2-7).

```
housing.describe()
```

	longitude	latitude	housing_median_age	total_rooms	total_bedrooms	median_house_value
count	20640.000000	20640.000000	20640.000000	20640.000000	20433.000000	20640.000000
mean	-119.569704	35.631861	28.639486	2635.763081	537.870553	206855.816909
std	2.003532	2.135952	12.585558	2181.615252	421.385070	115395.615874
min	-124.350000	32.540000	1.000000	2.000000	1.000000	14999.000000
25%	-121.800000	33.930000	18.000000	1447.750000	296.000000	119600.000000
50%	-118.490000	34.260000	29.000000	2127.000000	435.000000	179700.000000
75%	-118.010000	37.710000	37.000000	3148.000000	647.000000	264725.000000
max	-114.310000	41.950000	52.000000	39320.000000	6445.000000	500001.000000

Figure 2-7. Summary of each numerical attribute

The `count`, `mean`, `min`, and `max` rows are self-explanatory. Note that the null values are ignored (so, for example, the `count` of `total_bedrooms` is 20,433, not 20,640). The `std` row shows the *standard deviation*, which measures how dispersed the values are.[5] The 25%, 50%, and 75% rows show the corresponding *percentiles*: a percentile indicates the value below which a given percentage of observations in a group of observations fall. For example, 25% of the districts have a `housing_median_age` lower than 18, while 50% are lower than 29 and 75% are lower than 37. These are often called the 25th percentile (or first *quartile*), the median, and the 75th percentile (or third quartile).

Another quick way to get a feel of the type of data you are dealing with is to plot a histogram for each numerical attribute. A histogram shows the number of instances (on the vertical axis) that have a given value range (on the horizontal axis). You can either plot this one attribute at a time, or you can call the `hist()` method on the whole dataset (as shown in the following code example), and it will plot a histogram for each numerical attribute (see Figure 2-8):

```
import matplotlib.pyplot as plt

housing.hist(bins=50, figsize=(12, 8))
plt.show()
```

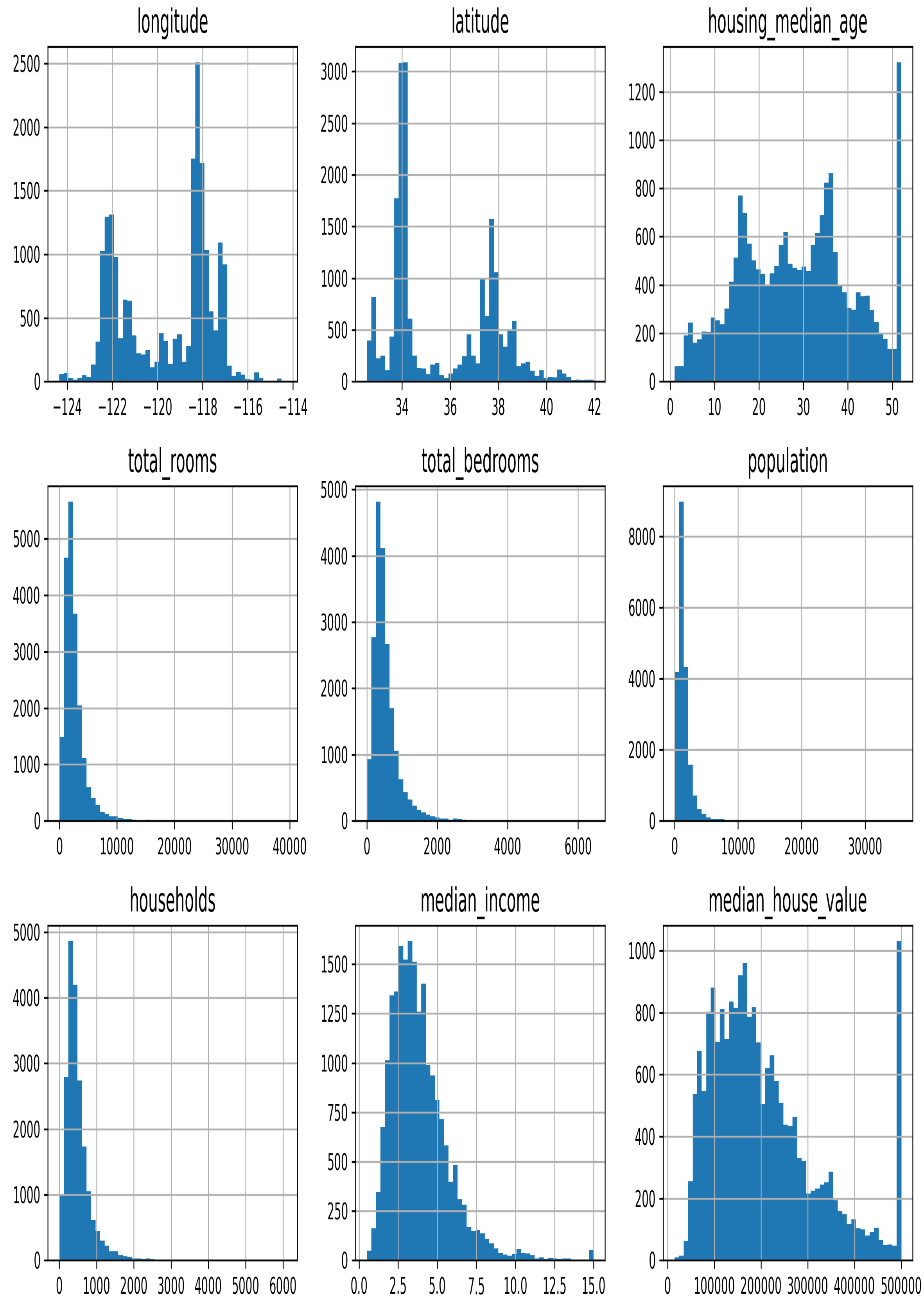


Figure 2-8. A histogram for each numerical attribute

There are a few things you might notice in these histograms:

1. First, the median income attribute does not look like it is expressed in US dollars (USD). After checking with the team that collected the data, you are told that the data has been scaled and capped at 15 (actually, 15.0001) for higher median incomes, and at 0.5 (actually, 0.4999) for lower median incomes. The numbers represent roughly tens of thousands of dollars (e.g., 3 actually means about $30,000). Working with preprocessed attributes is common in Machine Learning, and it is not necessarily a problem, but you should try to understand how the data was computed.

2. The housing median age and the median house value were also capped. The latter may be a serious problem since it is your target attribute (your labels). Your Machine Learning algorithms may learn that prices never go beyond that limit. You need to check with your client team (the team that will use your system's output) to see if this is a problem or not. If they tell you that they need precise predictions even beyond $500,000, then you have two options:

    a. Collect proper labels for the districts whose labels were capped.

    b. Remove those districts from the training set (and also from the test set, since your system should not be evaluated poorly if it predicts values beyond $500,000).

3. These attributes have very different scales. We will discuss this later in this chapter, when we explore feature scaling.

4. Finally, many histograms are *skewed right*: they extend much farther to the right of the median than to the left. This may make it a bit harder for some Machine Learning algorithms to detect patterns. We will try transforming these attributes later on to have more symmetrical and bell-shaped distributions.

Hopefully you now have a better understanding of the kind of data you are dealing with.

WARNING

Wait! Before you look at the data any further, you need to create a test set, put it aside, and never look at it.

Create a Test Set

It may sound strange to voluntarily set aside part of the data at this stage. After all, you have only taken a quick glance at the data, and surely you should learn a whole lot more about it before you decide what algorithms to use, right? This is true, but your brain is an amazing pattern detection system, which also means that it is highly prone to overfitting: if you look at the test set, you may stumble upon some seemingly interesting pattern in the test data that leads you to select a particular kind of Machine Learning model. When you estimate the generalization error using the test set, your estimate will be too optimistic, and you will launch a system that will not perform as well as expected. This is called *data snooping* bias.

Creating a test set is theoretically simple: pick some instances randomly, typically 20% of the dataset (or less if your dataset is very large), and set them aside:

```
import numpy as np

def shuffle_and_split_data(data, test_ratio):
    shuffled_indices = np.random.permutation(len(data))
    test_set_size = int(len(data) * test_ratio)
    test_indices = shuffled_indices[:test_set_size]
    train_indices = shuffled_indices[test_set_size:]
    return data.iloc[train_indices], data.iloc[test_indices]
```

You can then use this function like this:

```
>>> train_set, test_set = shuffle_and_split_data(housing, 0.2)
>>> len(train_set)
16512
>>> len(test_set)
4128
```

Well, this works, but it is not perfect: if you run the program again, it will generate a different test set! Over time, you (or your Machine Learning algorithms) will get to see the whole dataset, which is what you want to avoid.

One solution is to save the test set on the first run and then load it in subsequent runs. Another option is to set the random number generator's seed (e.g., with `np.random.seed(42)`)[6] before calling `np.random.permutation()` so that it always generates the same shuffled indices.

But both these solutions will break the next time you fetch an updated dataset. To have a stable train/test split even after updating the dataset, a common solution is to use each instance's identifier to decide whether or not it should go in the test set (assuming instances have a unique and immutable identifier). For example, you could compute a hash of each instance's identifier and put that instance in the test set if the hash is lower than or equal to 20% of the maximum hash value. This ensures that the test set will remain consistent across multiple runs, even if you refresh the dataset. The new test set will contain 20% of the new instances, but it will not contain any instance that was previously in the training set.

Here is a possible implementation:

```
from zlib import crc32

def is_id_in_test_set(identifier, test_ratio):
    return crc32(np.int64(identifier)) < test_ratio * 2**32

def split_data_with_id_hash(data, test_ratio, id_column):
    ids = data[id_column]
    in_test_set = ids.apply(lambda id_: is_id_in_test_set(id_,
test_ratio))
    return data.loc[~in_test_set], data.loc[in_test_set]
```

Unfortunately, the housing dataset does not have an identifier column. The simplest solution is to use the row index as the ID:

```
housing_with_id = housing.reset_index()  # adds an `index` column
train_set, test_set = split_data_with_id_hash(housing_with_id, 0.2,
"index")
```

If you use the row index as a unique identifier, you need to make sure that new data gets appended to the end of the dataset and that no row ever gets deleted. If this is not possible, then you can try to use the most stable features to build a unique identifier. For example, a district's latitude and longitude are guaranteed to be stable for a few million years, so you could combine them into an ID like so:[7]

```
housing_with_id["id"] = housing["longitude"] * 1000 +
housing["latitude"]
train_set, test_set = split_data_with_id_hash(housing_with_id, 0.2,
"id")
```

Scikit-Learn provides a few functions to split datasets into multiple subsets in various ways. The simplest function is `train_test_split()`, which does pretty much the same thing as the function `shuffle_and_split_data()` we defined earlier, with a couple of additional features. First, there is a `random_state` parameter that allows you to set the random generator seed. Second, you can pass it multiple datasets with an identical number of rows, and it will split them on the same indices (this is very useful, for example, if you have a separate DataFrame for labels):

```
from sklearn.model_selection import train_test_split

train_set, test_set = train_test_split(housing, test_size=0.2,
random_state=42)
```

So far we have considered purely random sampling methods. This is generally fine if your dataset is large enough (especially relative to the number of attributes), but if it is not, you run the risk of introducing a significant sampling bias. When a survey company decides to call 1,000 people to ask them a few questions, they don't just pick 1,000 people randomly in a phone book. They try to ensure that these 1,000 people are representative of the whole population, with regards to the questions they want to ask. For example, the US population is 51.1% females and 48.9% males, so a well-conducted survey in the US would try to maintain this ratio in the sample: 511 female and 489 male (at least if we believe that the answers may vary across genders). This is called *stratified sampling*: the population is divided into homogeneous subgroups called *strata*, and the right number of instances are sampled from each stratum to guarantee that the test set is representative of the overall population. If the people running the survey used purely random sampling, there would be about 10.7% chance of sampling a skewed test set with less than 48.5% female or more than 53.5% female. Either way, the survey results would likely be quite biased.

Suppose you chatted with experts who told you that the median income is a very important attribute to predict median housing prices. You may want to ensure that the test set is representative of the various categories of incomes in the whole dataset. Since the median income is a continuous numerical attribute, you first need to create an income category attribute. Let's look at the median income histogram more closely (back in Figure 2-8): most median income values are clustered around 1.5 to 6 (i.e., $15,000–$60,000), but some median incomes go far beyond 6. It is important to have a sufficient number of instances in your dataset for each stratum, or else the estimate of a stratum's importance may be biased. This means that you should not have too many strata, and each stratum should be large enough. The following code uses the `pd.cut()` function to create an income category attribute with five categories (labeled from 1 to 5): category 1 ranges from 0 to 1.5 (i.e., less than $15,000), category 2 from 1.5 to 3, and so on:

```
housing["income_cat"] = pd.cut(housing["median_income"],
                               bins=[0., 1.5, 3.0, 4.5, 6., np.inf],
                               labels=[1, 2, 3, 4, 5])
```

These income categories are represented in Figure 2-9:

```
housing["income_cat"].value_counts().sort_index().plot.bar(rot=0,
grid=True)
plt.xlabel("Income category")
plt.ylabel("Number of districts")
plt.show()
```

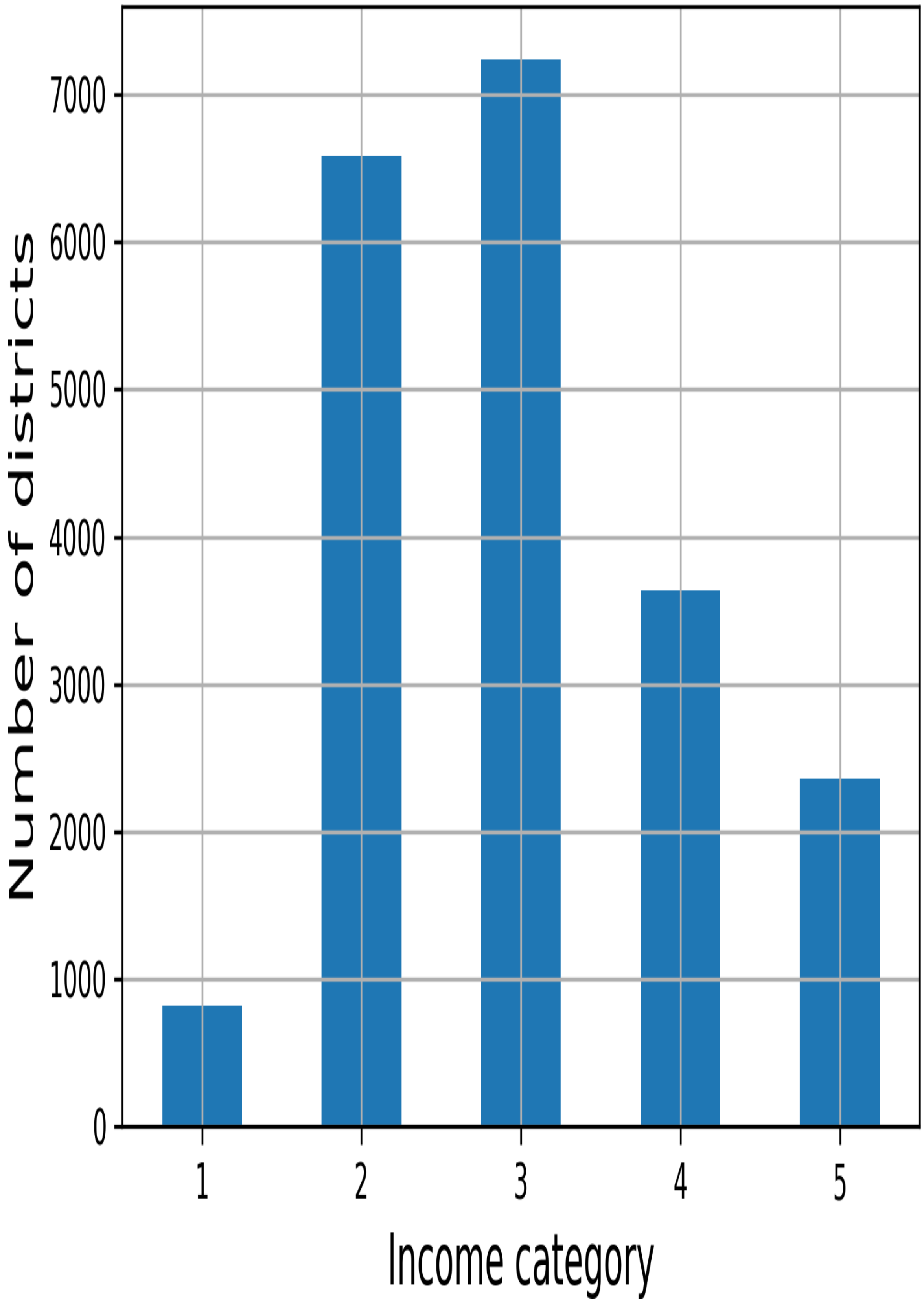


Figure 2-9. Histogram of income categories

Now you are ready to do stratified sampling based on the income category. Scikit-Learn provides a number of splitter classes in the `sklearn.model_selection` package, which implement various strategies to split your dataset into a train set and a test set. Each splitter has a `split()` method which returns an iterator over different train/test splits of the same data. To be precise, the `split()` method yields the train and test *indices*, not the data itself. Having multiple splits can be useful if you want to better estimate the performance of your model, as we will see when we discuss cross-validation later in this chapter. For example, the following code generates 10 different stratified splits of the same dataset:

```
from sklearn.model_selection import StratifiedShuffleSplit

splitter = StratifiedShuffleSplit(n_splits=10, test_size=0.2,
random_state=42)
strat_splits = []
for train_index, test_index in splitter.split(housing,
housing["income_cat"]):
    strat_train_set_n = housing.loc[train_index]
    strat_test_set_n = housing.loc[test_index]
    strat_splits.append([strat_train_set_n, strat_test_set_n])
```

For now, we can just use the first split:

```
strat_train_set, strat_test_set = strat_splits[0]
```

Since stratified sampling is fairly common, there's a shorter way to get a single split using the `train_test_split()` function with the `stratify` argument:

```
strat_train_set, strat_test_set = train_test_split(
    housing, test_size=0.2, stratify=housing["income_cat"],
random_state=42)
```

Let's see if this worked as expected. You can start by looking at the income category proportions in the test set:

```
>>> strat_test_set["income_cat"].value_counts() / len(strat_test_set)
3    0.350533
2    0.318798
4    0.176357
```

```
5    0.114341
1    0.039971
Name: income_cat, dtype: float64
```

With similar code you can measure the income category proportions in the full dataset. Figure 2-10 compares the income category proportions in the overall dataset, in the test set generated with stratified sampling, and in a test set generated using purely random sampling. As you can see, the test set generated using stratified sampling has income category proportions almost identical to those in the full dataset, whereas the test set generated using purely random sampling is skewed.

Income Category	Overall %	Stratified %	Random %	Strat. Error %	Rand. Error %
1	3.98	4.00	4.24	0.36	6.45
2	31.88	31.88	30.74	-0.02	-3.59
3	35.06	35.05	34.52	-0.01	-1.53
4	17.63	17.64	18.41	0.03	4.42
5	11.44	11.43	12.09	-0.08	5.63

Figure 2-10. Sampling bias comparison of stratified versus purely random sampling

Now we won't use the `income_cat` column anymore so we might as well drop it, reverting the data back to its original state:

```
for set_ in (strat_train_set, strat_test_set):
    set_.drop("income_cat", axis=1, inplace=True)
```

We spent quite a bit of time on test set generation for a good reason: this is an often neglected but critical part of a Machine Learning project. Moreover, many of these ideas will be useful later when we discuss cross-validation. Now it's time to move on to the next stage: exploring the data.

Discover and Visualize the Data to Gain Insights

So far you have only taken a quick glance at the data to get a general understanding of the kind of data you are manipulating. Now the goal is to go into a little more depth.

First, make sure you have put the test set aside and you are only exploring the training set. Also, if the training set is very large, you may want to sample an exploration set, to make manipulations easy and fast during the exploration phase. In our case, the training set is quite small, so we can just work directly on the full set. Since you're going to experiment with various transformations of the training set, you should make a copy of the original so you can revert to it afterwards:

```
housing = strat_train_set.copy()
```

Visualizing Geographical Data

Since there is geographical information (latitude and longitude), it is a good idea to create a scatterplot of all districts to visualize the data (Figure 2-11):

```
housing.plot(kind="scatter", x="longitude", y="latitude", grid=True)
plt.show()
```

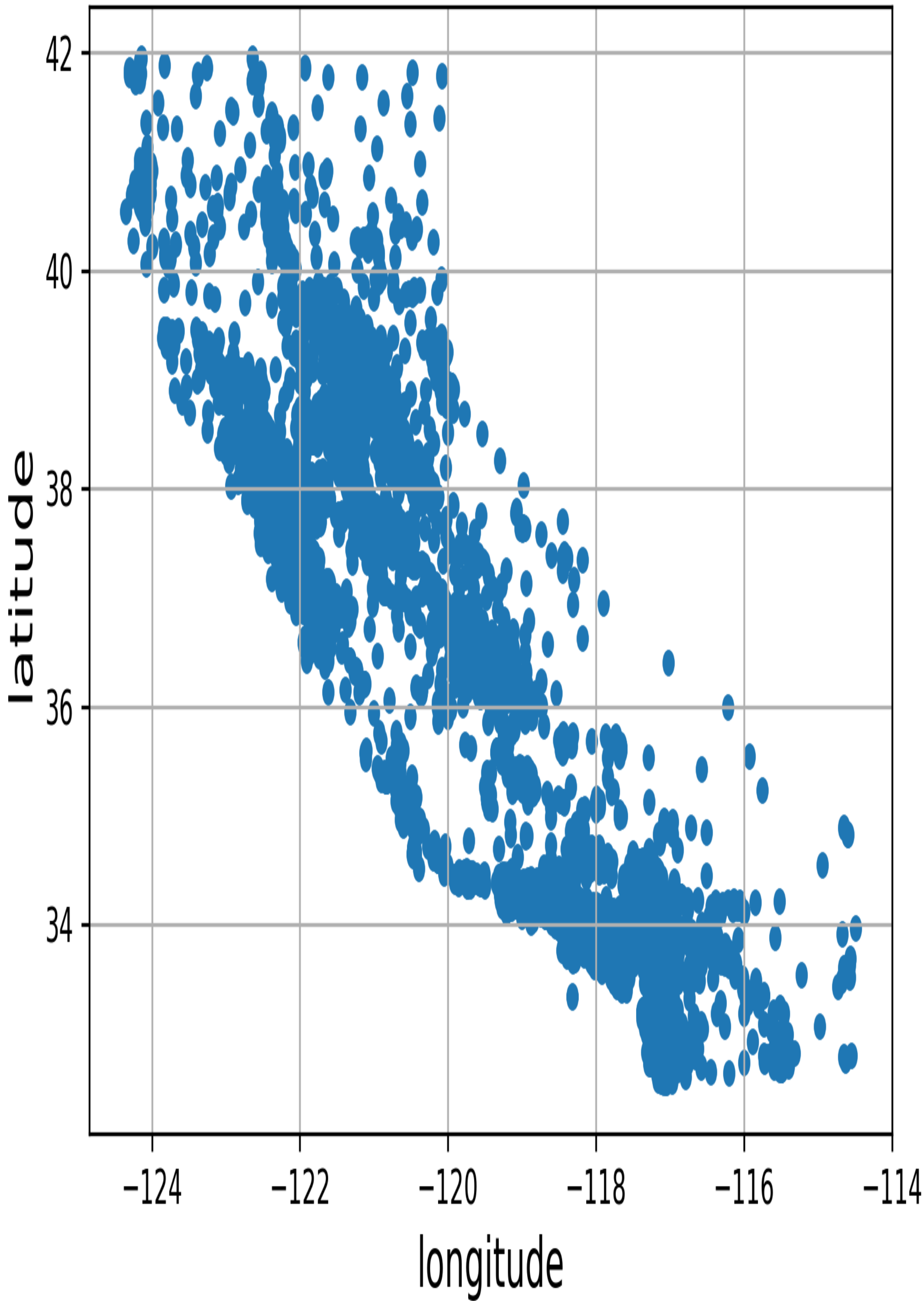


Figure 2-11. A geographical scatterplot of the data

This looks like California all right, but other than that it is hard to see any particular pattern. Setting the `alpha` option to `0.2` makes it much easier to visualize the places where there is a high density of data points (Figure 2-12):

```
housing.plot(kind="scatter", x="longitude", y="latitude", grid=True,
alpha=0.2)
plt.show()
```

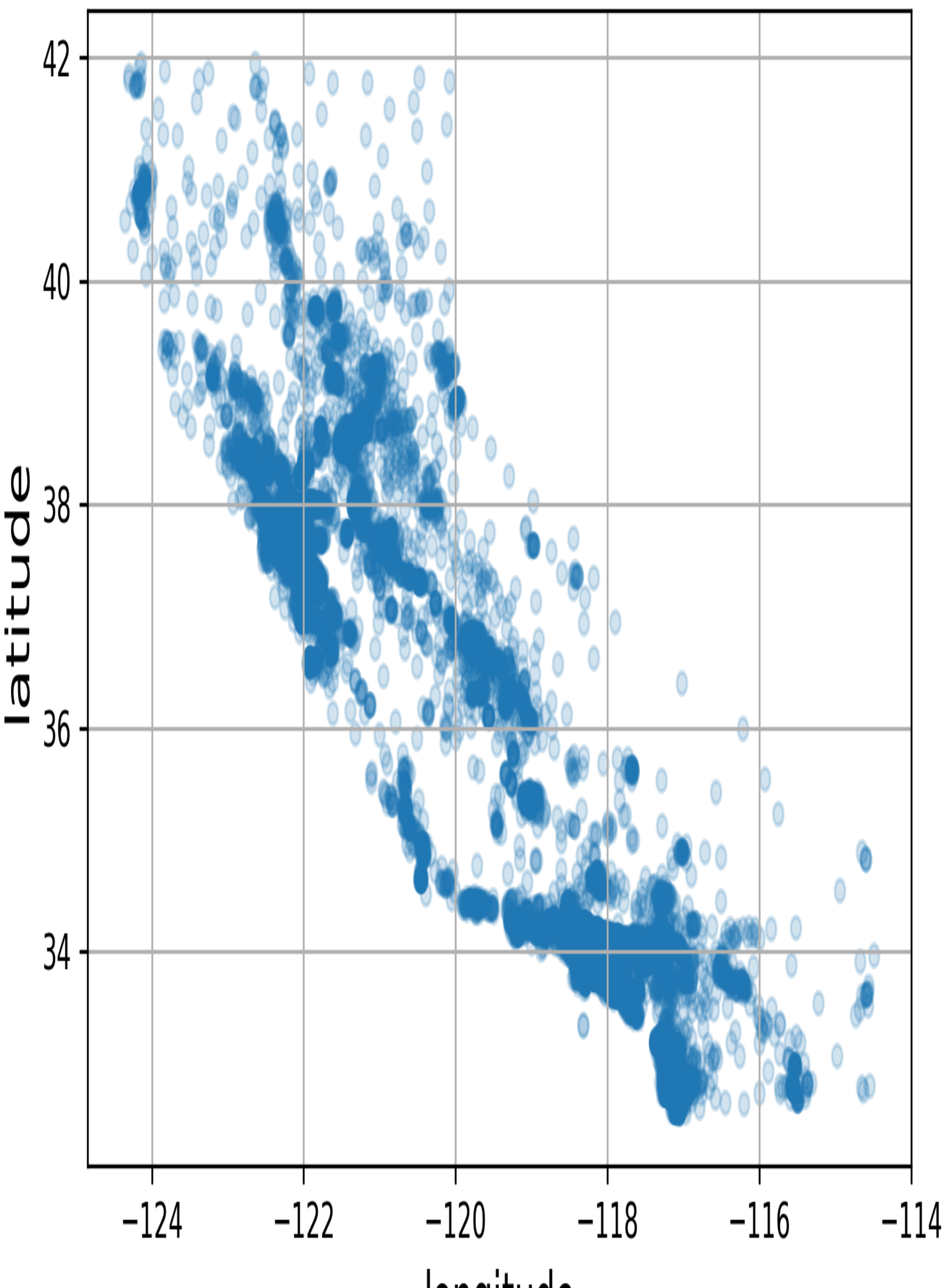


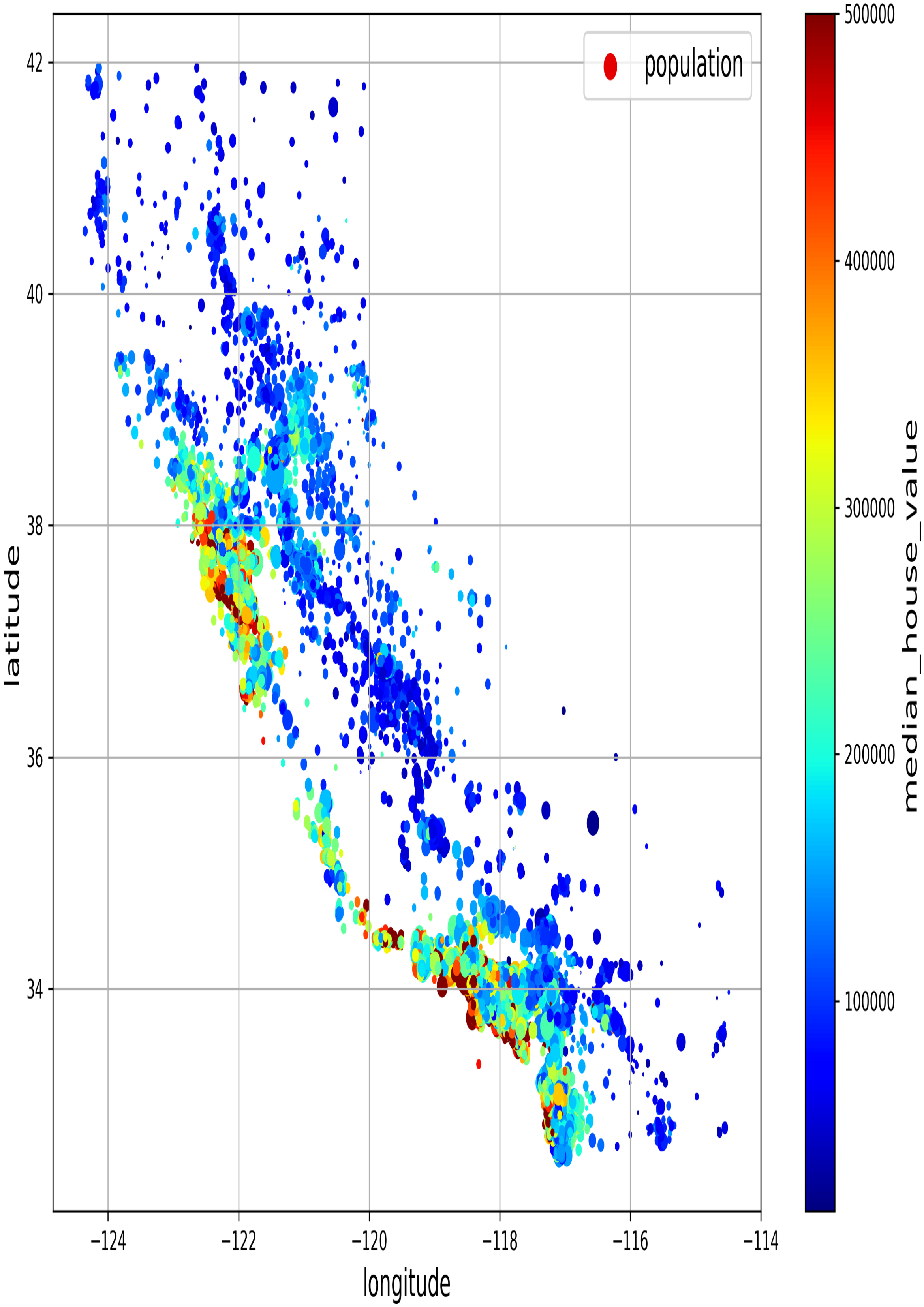
Figure 2-12. A better visualization that highlights high-density areas

Now that's much better: you can clearly see the high-density areas, namely the Bay Area and around Los Angeles and San Diego, plus a long line of fairly high density in the Central Valley, in particular around Sacramento and Fresno.

Our brains are very good at spotting patterns in pictures, but you may need to play around with visualization parameters to make the patterns stand out.

Now let's look at the housing prices (Figure 2-13). The radius of each circle represents the district's population (option `s`), and the color represents the price (option `c`). We will use a predefined color map (option `cmap`) called `jet`, which ranges from blue (low values) to red (high prices):[8]

```
housing.plot(kind="scatter", x="longitude", y="latitude", grid=True,
             s=housing["population"] / 100, label="population",
             c="median_house_value", cmap="jet", colorbar=True,
             legend=True, sharex=False, figsize=(10, 7))
plt.show()
```



population
latitude
longitude
median_house_value
42
40
38
36
34
−124
−122
−120
−118
−116
−114
500000
400000
300000
200000
100000

Figure 2-13. California housing prices: red is expensive, blue is cheap, larger circles indicate areas with a larger population

This image tells you that the housing prices are very much related to the location (e.g., close to the ocean) and to the population density, as you probably knew already. A clustering algorithm should be useful for detecting the main cluster and for adding new features that measure the proximity to the cluster centers. The ocean proximity attribute may be useful as well, although in Northern California the housing prices in coastal districts are not too high, so it is not a simple rule.

Looking for Correlations

Since the dataset is not too large, you can easily compute the *standard correlation coefficient* (also called *Pearson's r*) between every pair of attributes using the `corr()` method:

```
corr_matrix = housing.corr()
```

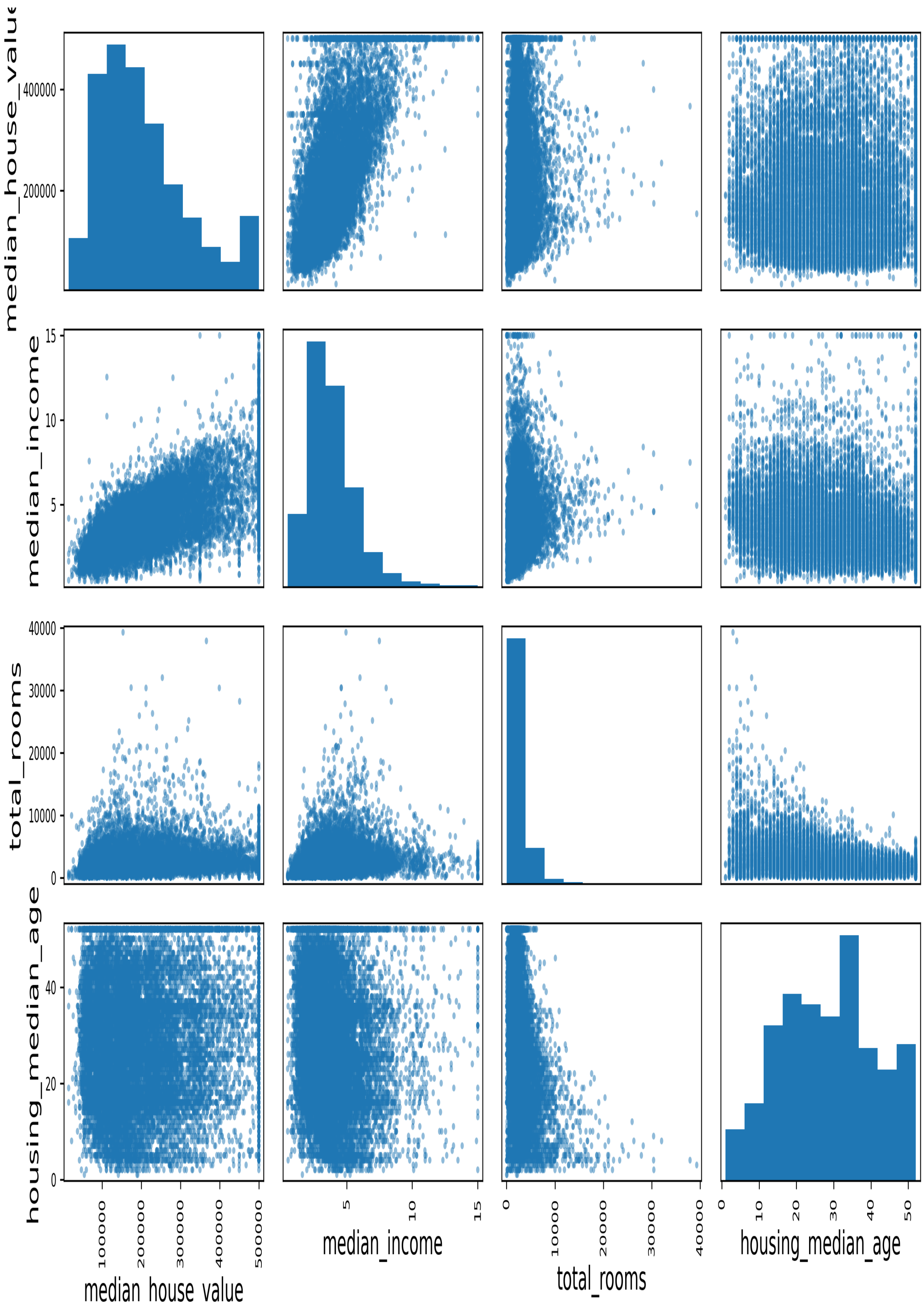
Now let's look at how much each attribute correlates with the median house value:

```
>>> corr_matrix["median_house_value"].sort_values(ascending=False)
median_house_value    1.000000
median_income         0.688380
total_rooms           0.137455
housing_median_age    0.102175
households            0.071426
total_bedrooms        0.054635
population           -0.020153
longitude            -0.050859
latitude             -0.139584
Name: median_house_value, dtype: float64
```

The correlation coefficient ranges from –1 to 1. When it is close to 1, it means that there is a strong positive correlation; for example, the median house value tends to go up when the median income goes up. When the coefficient is close to –1, it means that there is a strong negative correlation; you can see a small negative correlation between the latitude and the median house value (i.e., prices have a slight tendency to go down when you go north). Finally, coefficients close to 0 mean that there is no linear correlation.

Another way to check for correlation between attributes is to use the Pandas `scatter_matrix()` function, which plots every numerical attribute against every other numerical attribute. Since there are now 11 numerical attributes, you would get $11^2 = 121$ plots, which would not fit on a page—so let's just focus on a few promising attributes that seem most correlated with the median housing value (Figure 2-14):

```
from pandas.plotting import scatter_matrix

attributes = ["median_house_value", "median_income", "total_rooms",
              "housing_median_age"]
scatter_matrix(housing[attributes], figsize=(12, 8))
plt.show()
```



median_house_value
median_income
total_rooms
housing_median_age
400000
200000
15
10
5
40000
30000
20000
10000
0
40
20
0
100000
200000
300000
400000
500000
5
10
15
0
10000
20000
30000
40000
0
10
20
30
40
50
median_house_value
median_income
total_rooms
housing_median_age

Figure 2-14. This scatter matrix plots every numerical attribute against every other numerical attribute, plus a histogram of each numerical attribute's values on the main diagonal (top left to bottom right)

The main diagonal would be full of straight lines if Pandas plotted each variable against itself, which would not be very useful. So instead Pandas displays a histogram of each attribute (other options are available; see Pandas' documentation for more details).

Looking at the correlation scatterplots, it seems like the most promising attribute to predict the median house value is the median income, so let's zoom in on their scatterplot (Figure 2-15):

```
housing.plot(kind="scatter", x="median_income",
y="median_house_value",
             alpha=0.1, grid=True)
plt.show()
```

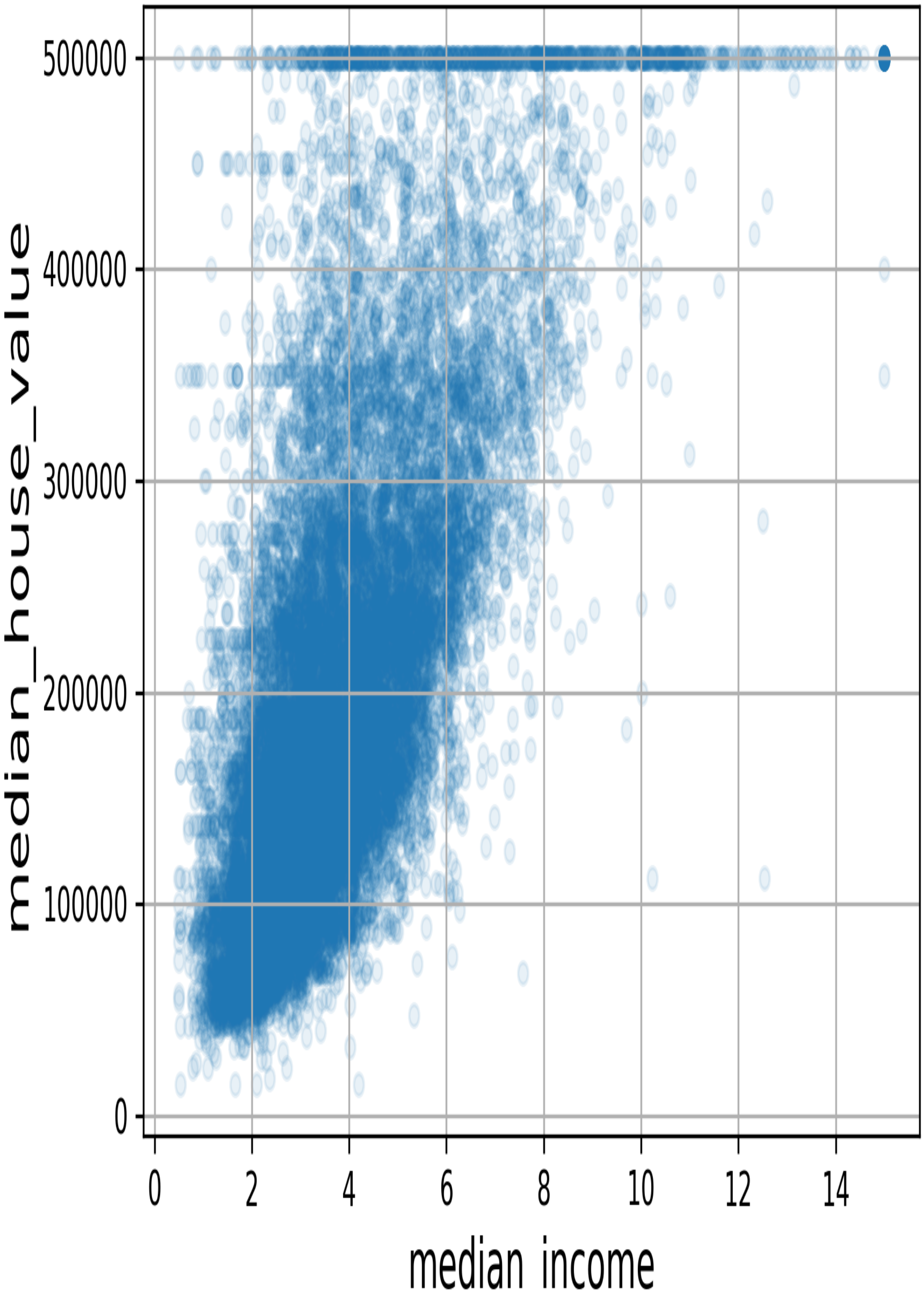


Figure 2-15. Median income versus median house value

This plot reveals a few things. First, the correlation is indeed quite strong; you can clearly see the upward trend, and the points are not too dispersed. Second, the price cap that we noticed earlier is clearly visible as a horizontal line at $500,000. But this plot reveals other less obvious straight lines: a horizontal line around $450,000, another around $350,000, perhaps one around $280,000, and a few more below that. You may want to try removing the corresponding districts to prevent your algorithms from learning to reproduce these data quirks.

WARNING

The correlation coefficient only measures linear correlations ("as *x* goes up, *y* generally goes up/down"). It may completely miss out on nonlinear relationships (e.g., "as *x* approaches 0, *y* generally goes up"). Figure 2-16 shows a variety of datasets along with their correlation coefficient. Note how all the plots of the bottom row have a correlation coefficient equal to 0, despite the fact that their axes are clearly *not* independent: these are examples of nonlinear relationships. Also, the second row shows examples where the correlation coefficient is equal to 1 or –1; notice that this has nothing to do with the slope. For example, your height in inches has a correlation coefficient of 1 with your height in feet or in nanometers.

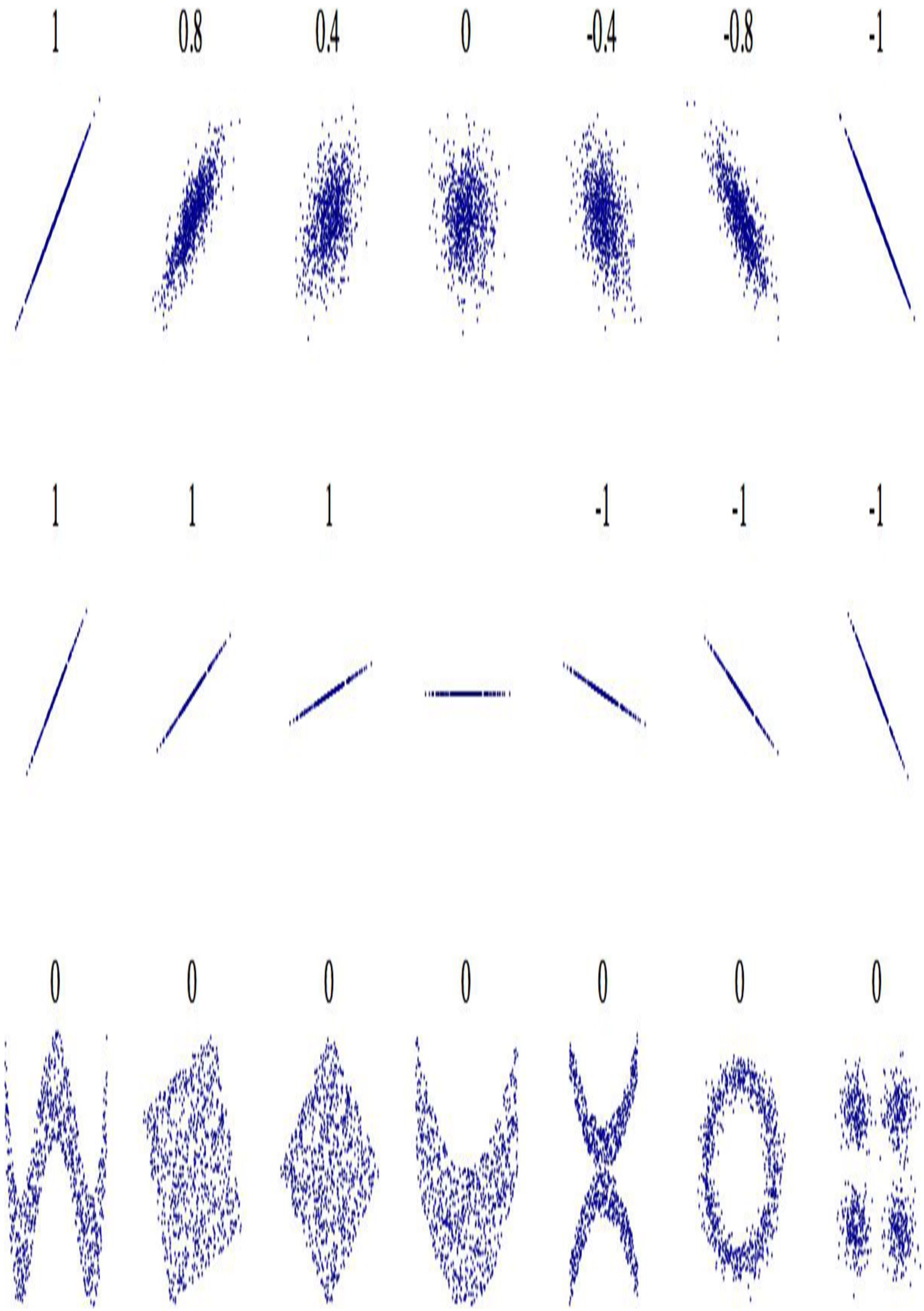

1 0.8 0.4 0 -0.4 -0.8 -1
1 1 1 -1 -1 -1
0 0 0 0 0 0 0

Figure 2-16. Standard correlation coefficient of various datasets (source: Wikipedia; public domain image)

Experimenting with Attribute Combinations

Hopefully the previous sections gave you an idea of a few ways you can explore the data and gain insights. You identified a few data quirks that you may want to clean up before feeding the data to a Machine Learning algorithm, and you found interesting correlations between attributes, in particular with the target attribute. You also noticed that some attributes have a skewed-right distribution, so you may want to transform them (e.g., by computing their logarithm or square root). Of course, your mileage will vary considerably with each project, but the general ideas are similar.

One last thing you may want to do before preparing the data for Machine Learning algorithms is to try out various attribute combinations. For example, the total number of rooms in a district is not very useful if you don't know how many households there are. What you really want is the number of rooms per household. Similarly, the total number of bedrooms by itself is not very useful: you probably want to compare it to the number of rooms. And the population per household also seems like an interesting attribute combination to look at. Let's create these new attributes:

```
housing["rooms_per_house"] = housing["total_rooms"] /
housing["households"]
housing["bedrooms_ratio"] = housing["total_bedrooms"] /
housing["total_rooms"]
housing["people_per_house"] = housing["population"] /
housing["households"]
```

And now let's look at the correlation matrix again:

```
>>> corr_matrix = housing.corr()
>>> corr_matrix["median_house_value"].sort_values(ascending=False)
median_house_value    1.000000
median_income         0.688380
rooms_per_house       0.143663
total_rooms           0.137455
housing_median_age    0.102175
households            0.071426
total_bedrooms        0.054635
population           -0.020153
```

```
people_per_house      -0.038224
longitude             -0.050859
latitude              -0.139584
bedrooms_ratio        -0.256397
Name: median_house_value, dtype: float64
```

Hey, not bad! The new `bedrooms_ratio` attribute is much more correlated with the median house value than the total number of rooms or bedrooms. Apparently houses with a lower bedroom/room ratio tend to be more expensive. The number of rooms per household is also more informative than the total number of rooms in a district—obviously the larger the houses, the more expensive they are.

This round of exploration does not have to be absolutely thorough; the point is to start off on the right foot and quickly gain insights that will help you get a first reasonably good prototype. But this is an iterative process: once you get a prototype up and running, you can analyze its output to gain more insights and come back to this exploration step.

Prepare the Data for Machine Learning Algorithms

It's time to prepare the data for your Machine Learning algorithms. Instead of doing this manually, you should write functions for this purpose, for several good reasons:

- This will allow you to reproduce these transformations easily on any dataset (e.g., the next time you get a fresh dataset).
- You will gradually build a library of transformation functions that you can reuse in future projects.
- You can use these functions in your live system to transform the new data before feeding it to your algorithms.
- This will make it possible for you to easily try various transformations and see which combination of transformations works best.

But first let's revert to a clean training set (by copying `strat_train_set` once again). Let's also separate the predictors and the labels, since we don't necessarily want to apply the same transformations to the predictors and the target values (note that `drop()` creates a copy of the data and does not affect `strat_train_set`):

```
housing = strat_train_set.drop("median_house_value", axis=1)
housing_labels = strat_train_set["median_house_value"].copy()
```

Data Cleaning

Most Machine Learning algorithms cannot work with missing features, so let's create a few functions to take care of them. We saw earlier that the `total_bedrooms` attribute has some missing values, so let's fix this. You have three options:

1. Get rid of the corresponding districts.
2. Get rid of the whole attribute.
3. Set the missing values to some value (zero, the mean, the median, etc.). This is called *imputation*.

You can accomplish these easily using DataFrame's `dropna()`, `drop()`, and `fillna()` methods:

```
housing.dropna(subset=["total_bedrooms"], inplace=True)   # option 1

housing.drop("total_bedrooms", axis=1)   # option 2

median = housing["total_bedrooms"].median()   # option 3
housing["total_bedrooms"].fillna(median, inplace=True)
```

Let's go for option 3 since it is the least destructive, but instead of the code above, we will use a handy Scikit-Learn class : `SimpleImputer`. The benefit is that it will store the median value of each feature: this will make it possible to impute missing values not only on the training set, but also on the validation set, the test set, and any new data fed to the model. Here is how to use it. First, you need to create a `SimpleImputer` instance, specifying that you want to replace each attribute's missing values with the median of that attribute:

```
from sklearn.impute import SimpleImputer

imputer = SimpleImputer(strategy="median")
```

Since the median can only be computed on numerical attributes, you need to create a copy of the data with only the numerical attributes (this will exclude the text attribute `ocean_proximity`):

```
housing_num = housing.select_dtypes(include=[np.number])
```

Now you can fit the `imputer` instance to the training data using the `fit()` method:

```
imputer.fit(housing_num)
```

The `imputer` has simply computed the median of each attribute and stored the result in its `statistics_` instance variable. Only the `total_bedrooms` attribute had missing values, but we cannot be sure that there won't be any missing values in new data after the system goes live, so it is safer to apply the `imputer` to all the numerical attributes:

```
>>> imputer.statistics_
array([-118.51 , 34.26 , 29. , 2125. , 434. , 1167. , 408. , 3.5385])
>>> housing_num.median().values
array([-118.51 , 34.26 , 29. , 2125. , 434. , 1167. , 408. , 3.5385])
```

Now you can use this "trained" `imputer` to transform the training set by replacing missing values with the learned medians:

```
X = imputer.transform(housing_num)
```

Missing values can also be replaced with the mean value (`strategy="mean"`), or with the most frequent value (`strategy="most_frequent"`), or with a constant value (`strategy="constant", fill_value=…`). The last two strategies support non-numerical data.

TIP

There are also more powerful imputers available in the `sklearn.impute` package (both for numerical features only):

- `KNNImputer` replaces each missing value with the mean of the *k* nearest neighbors' values for that feature. The distance is based on all the available features.
- `IterativeImputer` trains a regression model per feature to predict the missing values based on all the other available features. It then trains the model again on the updated data, and repeats the process several times, improving the models and the replacement values at each iteration.

SCIKIT-LEARN DESIGN

Scikit-Learn's API is remarkably well designed. These are the main design principles:[9]

Consistency

All objects share a consistent and simple interface:

Estimators

Any object that can estimate some parameters based on a dataset is called an *estimator* (e.g., a `SimpleImputer` is an estimator). The estimation itself is performed by the `fit()` method, and it takes a dataset as a parameter, or two for supervised learning algorithms—the second dataset contains the labels. Any other parameter needed to guide the estimation process is considered a hyperparameter (such as a `SimpleImputer`'s `strategy`), and it must be set as an instance variable (generally via a constructor parameter).

Transformers

Some estimators (such as a `SimpleImputer`) can also transform a dataset; these are called *transformers*. Once again, the API is simple: the transformation is performed by the `transform()` method with the dataset to transform as a parameter. It returns the transformed dataset. This transformation generally relies on the learned parameters, as is the case for a `SimpleImputer`. All transformers also have a convenience method called `fit_transform()` which is equivalent to calling `fit()` and then `transform()` (but sometimes `fit_transform()` is optimized and runs much faster).

Predictors

Finally, some estimators, given a dataset, are capable of making predictions; they are called *predictors*. For example, the `LinearRegression` model in the previous chapter was a predictor: given a country's GDP per capita, it predicted life satisfaction. A predictor has a `predict()` method that takes a dataset of new instances and returns a dataset of corresponding predictions. It also has a `score()` method that measures the quality of the predictions, given a test set (and the corresponding labels, in the case of supervised learning algorithms).{wj}[10]

Inspection

All the estimator's hyperparameters are accessible directly via public instance variables (e.g., `imputer.strategy`), and all the estimator's learned parameters are accessible via public instance variables with an underscore suffix (e.g., `imputer.statistics_`).

Nonproliferation of classes

Datasets are represented as NumPy arrays or SciPy sparse matrices, instead of homemade classes. Hyperparameters are just regular Python strings or numbers.

Composition

Existing building blocks are reused as much as possible. For example, it is easy to create a `Pipeline` estimator from an arbitrary sequence of transformers followed by a final estimator, as we will see.

Sensible defaults

Scikit-Learn provides reasonable default values for most parameters, making it easy to quickly create a baseline working system.

Scikit-Learn transformers output NumPy arrays (or sometimes SciPy sparse matrices) even when they are fed Pandas DataFrames as input.[11] So the output of `imputer.transform(housing_num)` is a NumPy array: `X` has neither column names nor index. Luckily, it's not too hard to wrap `X` in a DataFrame and recover the column names and index from `housing_num`:

```
housing_tr = pd.DataFrame(X, columns=housing_num.columns,
                          index=housing_num.index)
```

Handling Text and Categorical Attributes

So far we have only dealt with numerical attributes, but now let’s look at text attributes. In this dataset, there is just one: the `ocean_proximity` attribute. Let’s look at its value for the first few instances:

```
>>> housing_cat = housing[["ocean_proximity"]]
>>> housing_cat.head(8)
      ocean_proximity
13096        NEAR BAY
14973       <1H OCEAN
3785           INLAND
14689          INLAND
20507      NEAR OCEAN
1286           INLAND
18078       <1H OCEAN
4396         NEAR BAY
```

It’s not arbitrary text: there are a limited number of possible values, each of which represents a category. So this attribute is a categorical attribute. Most Machine Learning algorithms prefer to work with numbers, so let’s convert these categories from text to numbers. For this, we can use Scikit-Learn’s `OrdinalEncoder` class:

```
from sklearn.preprocessing import OrdinalEncoder

ordinal_encoder = OrdinalEncoder()
housing_cat_encoded = ordinal_encoder.fit_transform(housing_cat)
```

Here’s what the first few encoded values in `housing_cat_encoded` look like:

```
>>> housing_cat_encoded[:8]
array([[3.],
       [0.],
       [1.],
       [1.],
       [4.],
       [1.],
```

```
       [0.],
       [3.]])
```

You can get the list of categories using the `categories_` instance variable. It is a list containing a 1D array of categories for each categorical attribute (in this case, a list containing a single array since there is just one categorical attribute):

```
>>> ordinal_encoder.categories_
[array(['<1H OCEAN', 'INLAND', 'ISLAND', 'NEAR BAY', 'NEAR OCEAN'],
       dtype=object)]
```

One issue with this representation is that ML algorithms will assume that two nearby values are more similar than two distant values. This may be fine in some cases (e.g., for ordered categories such as "bad," "average," "good," and "excellent"), but it is obviously not the case for the `ocean_proximity` column (for example, categories 0 and 4 are clearly more similar than categories 0 and 1). To fix this issue, a common solution is to create one binary attribute per category: one attribute equal to 1 when the category is "<1H OCEAN" (and 0 otherwise), another attribute equal to 1 when the category is "INLAND" (and 0 otherwise), and so on. This is called *one-hot encoding*, because only one attribute will be equal to 1 (hot), while the others will be 0 (cold). The new attributes are sometimes called *dummy* attributes. Scikit-Learn provides a `OneHotEncoder` class to convert categorical values into one-hot vectors:

```
from sklearn.preprocessing import OneHotEncoder

cat_encoder = OneHotEncoder()
housing_cat_1hot = cat_encoder.fit_transform(housing_cat)
```

By default, the output of a `OneHotEncoder` is a SciPy *sparse matrix*, instead of a NumPy array:

```
>>> housing_cat_1hot
<16512x5 sparse matrix of type '<class 'numpy.float64'>'
 with 16512 stored elements in Compressed Sparse Row format>
```

A sparse matrix is a very efficient representation for matrices that contain mostly zeroes. Indeed, internally it only stores the non-zero values and their positions. When a categorical attribute has hundreds or thousands of categories, then one-hot-encoding it results in a very large matrix full of zeros except for a single 1 per row. In this case, a sparse matrix is exactly what we need: it will save plenty of memory and speed up computations. You can use a sparse matrix mostly like a normal 2D array,[12] but if you want to convert it to a (dense) NumPy array, just call the `toarray()` method:

```
>>> housing_cat_1hot.toarray()
array([[0., 0., 0., 1., 0.],
       [1., 0., 0., 0., 0.],
       [0., 1., 0., 0., 0.],
       ...,
       [0., 0., 0., 0., 1.],
       [1., 0., 0., 0., 0.],
       [0., 0., 0., 0., 1.]])
```

Alternatively, you can set `sparse=False` when creating the `OneHotEncoder`, in which case the `transform()` method will return a regular (dense) NumPy array directly.

As with the `OrdinalEncoder`, you can get the list of categories using the encoder's `categories_` instance variable:

```
>>> cat_encoder.categories_
[array(['<1H OCEAN', 'INLAND', 'ISLAND', 'NEAR BAY', 'NEAR OCEAN'],
       dtype=object)]
```

Pandas has a function called `get_dummies()` which also converts each categorical feature into a one-hot-representation, with one binary feature per category:

```
>>> df_test = pd.DataFrame({"ocean_proximity": ["INLAND", "NEAR
BAY"]})
>>> pd.get_dummies(df_test)
   ocean_proximity_INLAND  ocean_proximity_NEAR BAY
0                       1                         0
1                       0                         1
```

It looks nice and simple, so why not use it instead of `OneHotEncoder`? Well, the advantage of `OneHotEncoder` is that it remembers which categories it was trained on. This is very important because once your model is in production, it should be fed exactly the same features as during training: no more, no less. Watch what our trained `cat_encoder` outputs when we make it transform the same `df_test` (using `transform()`, not `fit_transform()`):

```
>>> cat_encoder.transform(df_test)
array([[0., 1., 0., 0., 0.],
       [0., 0., 0., 1., 0.]])
```

See the difference? `get_dummies()` saw only two categories, so it output two columns, whereas `OneHotEncoder` output one column per learned category, in the right order. Moreover, if you feed `get_dummies()` a DataFrame containing an unknown category (e.g., `"<2H OCEAN"`), it will happily generate a column for it:

```
>>> df_test_unknown = pd.DataFrame({"ocean_proximity": ["<2H OCEAN",
"ISLAND"]})
>>> pd.get_dummies(df_test_unknown)
   ocean_proximity_<2H OCEAN  ocean_proximity_ISLAND
0                          1                       0
1                          0                       1
```

But `OneHotEncoder` is smarter: it will detect the unknown category and raise an exception. If you prefer, you can set the `handle_unknown` hyperparameter to `"ignore"`, in which case it will just represent the unknown category with zeros:

```
>>> cat_encoder.handle_unknown = "ignore"
>>> cat_encoder.transform(df_test_unknown)
array([[0., 0., 0., 0., 0.],
       [0., 0., 1., 0., 0.]])
```

When you fit any Scikit-Learn estimator using a DataFrame, the estimator stores the column names in the `feature_names_in_` attribute. Scikit-Learn then ensures that any DataFrame fed to this estimator after that (e.g., to `transform()` or `predict()`) has the same column names. Transformers also provide a `get_feature_names_out()` method which you can use to build a DataFrame around the transformer's output:

```
>>> cat_encoder.feature_names_in_
array(['ocean_proximity'], dtype=object)
>>> cat_encoder.get_feature_names_out()
array(['ocean_proximity_<1H OCEAN', 'ocean_proximity_INLAND',
       'ocean_proximity_ISLAND', 'ocean_proximity_NEAR BAY',
       'ocean_proximity_NEAR OCEAN'], dtype=object)
>>> df_output = pd.DataFrame(cat_encoder.transform(df_test_unknown),
...
columns=cat_encoder.get_feature_names_out(),
...                          index=df_test_unknown.index)
...
```

> **TIP**
>
> If a categorical attribute has a large number of possible categories (e.g., country code, profession, species), then one-hot encoding will result in a large number of input features. This may slow down training and degrade performance. If this happens, you may want to replace the categorical input with useful numerical features related to the categories: for example, you could replace the `ocean_proximity` feature with the distance to the ocean (similarly, a country code could be replaced with the country's population and GDP per capita). Alternatively, you can use one of the encoders provided by the category_encoders package on *https://github.com/scikit-learn-contrib*. Or when dealing with neural networks, you can replace each category with a learnable, low-dimensional vector called an *embedding*. This is an example of *representation learning* (see Chapters 13 and 17 for more details).

Feature Scaling and Transformation

One of the most important transformations you need to apply to your data is *feature scaling*. With few exceptions, Machine Learning algorithms don't perform well when the input numerical attributes have very different scales. This is the case for the housing data: the total number of rooms ranges from about 6 to 39,320, while the median incomes only range from 0 to 15.

There are two common ways to get all attributes to have the same scale: *min-max scaling* and *standardization*.

Min-max scaling (many people call this *normalization*) is the simplest: for each attribute, the values are shifted and rescaled so that they end up ranging from 0 to 1. This is performed by subtracting the min value and dividing by the difference between the min and the max. Scikit-Learn provides a transformer called `MinMaxScaler` for this. It has a `feature_range` hyperparameter that lets you change the range if, for some reason, you don't want 0–1 (e.g., neural networks work best with zero-mean inputs, so a range of –1 to 1 is preferable). It's quite easy to use:

```
from sklearn.preprocessing import MinMaxScaler

min_max_scaler = MinMaxScaler(feature_range=(-1, 1))
housing_num_min_max_scaled =
min_max_scaler.fit_transform(housing_num)
```

> **WARNING**
>
> As with all estimators, it is important to fit the scalers to the training data only: never use `fit()` or `fit_transform()` for anything else than the training set. Once you have a trained scaler, you can then use it to `transform()` any other set, including the validation set, the test set, and new data. Note that while the training set values will always be scaled to the specified range, if new data contains outliers, these may end up scaled outside the range. If you want to avoid this, just set the `clip` hyperparameter to `True`.

Standardization is different: first it subtracts the mean value (so standardized values have a zero mean), then it divides the result by the standard deviation (so standardized values have a standard deviation equal to 1). Unlike min-max scaling, standardization does not bound values to a specific range. However, standardization is much less affected by outliers. For example, suppose a district has a median income equal to 100 (by mistake), instead of the usual 0–15. Min-max scaling to the 0–1 range would map this outlier down to 1 and it would crush all the other values down to 0–0.15, whereas standardization would not be much affected. Scikit-Learn provides a transformer called `StandardScaler` for standardization:

```
from sklearn.preprocessing import StandardScaler

std_scaler = StandardScaler()
housing_num_std_scaled = std_scaler.fit_transform(housing_num)
```

> **TIP**
>
> If you want to scale a sparse matrix without converting it to a dense matrix first, you can use a `StandardScaler` with its `with_mean` hyperparameter set to `False`: it will only divide the data by the standard deviation, without subtracting the mean (as this would break sparsity).

When a feature's distribution has a *heavy tail* (i.e., when values far from the mean are not exponentially rare), both min-max scaling and standardization will squash most values into a small range. Machine Learning models generally don't like this at all, as we will see in Chapter 4. So *before* you scale the feature, you should first transform it to shrink the heavy tail, and if possible to make the distribution roughly symmetrical. For example, a common way to do this for positive features with a heavy tail to the right is to replace the feature with its square root (or raise the feature to a power between 0 and 1). If the feature has a really long and heavy tail, such as a *power law distribution*, then replacing the feature with its logarithm may help. For example, the `population` feature roughly follows a power law: districts with 10,000 inhabitants are only 10 times less frequent than districts with 1,000 inhabitants, not exponentially less frequent. Figure 2-17 shows how much better this feature looks when you compute its log: it's very close to a Gaussian distribution (i.e., bell-shaped).

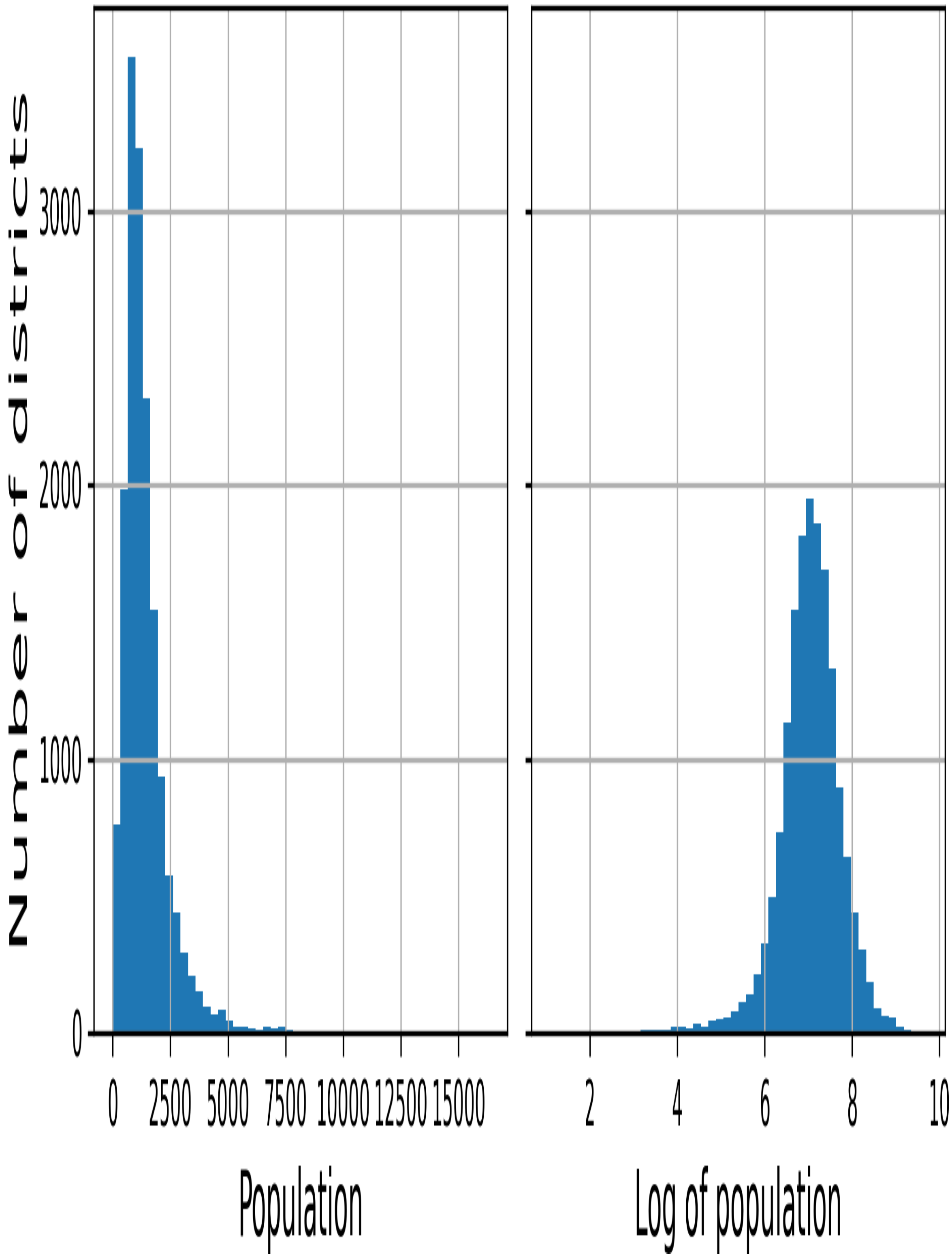


Figure 2-17. Transforming a feature to make it closer to a Gaussian distribution

Another approach to handle heavy tailed features consists in *bucketizing* the feature. This means chopping its distribution into roughly equal size buckets, and replacing each feature value with the index of the bucket it belongs to, much like we did to create the `income_cat` feature (although we only used it for stratified sampling). For example, you could replace each value with its percentile. Bucketizing with equal-sized buckets results in a feature with an almost uniform distribution, so there's no need for further scaling, or you can just divide by the number of buckets to force the values to the 0–1 range.

When a feature has a multimodal distribution (i.e., with two or more clear peaks, called *modes*), such as the `housing_median_age` feature, it can also be helpful to bucketize it, but this time treating the bucket ids as categories, rather than as numerical values. This means that the bucket indices must be encoded, for example using a `OneHotEncoder` (so you usually don't want to use too many buckets). This approach will allow the regression model to more easily learn different rules for different ranges of this feature value. For example, perhaps houses built around 35 years ago have a peculiar style that fell out of fashion, and therefore they're cheaper than their age alone would suggest.

Another approach for transforming multimodal distributions is to add a feature for each of the modes (at least the main ones), representing the similarity between the housing median age and that particular mode. The similarity measure is typically computed using a *Radial Basis Function* (RBF): this is any function which depends only on the distance between the input value and a fixed point. The most commonly used RBF is the Gaussian RBF whose output value decays exponentially as the input value moves away from the fixed point. For example, the Gaussian RBF similarity between the housing age *x* and 35 is given by the equation $\exp(-\gamma(x - 35)^2)$. The hyperparameter γ (gamma) determines how quickly the similarity measure decays as *x* moves away from 35. Using Scikit-Learn's `rbf_kernel()` function, we can create a new Gaussian RBF feature measuring the similarity between the housing median age and 35:

```
from sklearn.metrics.pairwise import rbf_kernel

age_simil_35 = rbf_kernel(housing[["housing_median_age"]], [[35]],
gamma=0.1)
```

Figure 2-18 shows this new feature as a function of the housing median age (solid line). It also shows what the feature would look like if we used a smaller `gamma` value. As the chart shows, the new age similarity feature peaks at 35, right around the spike in the housing median age distribution: if this particular age group is well correlated with lower prices, there's a good chance that this new feature will help.

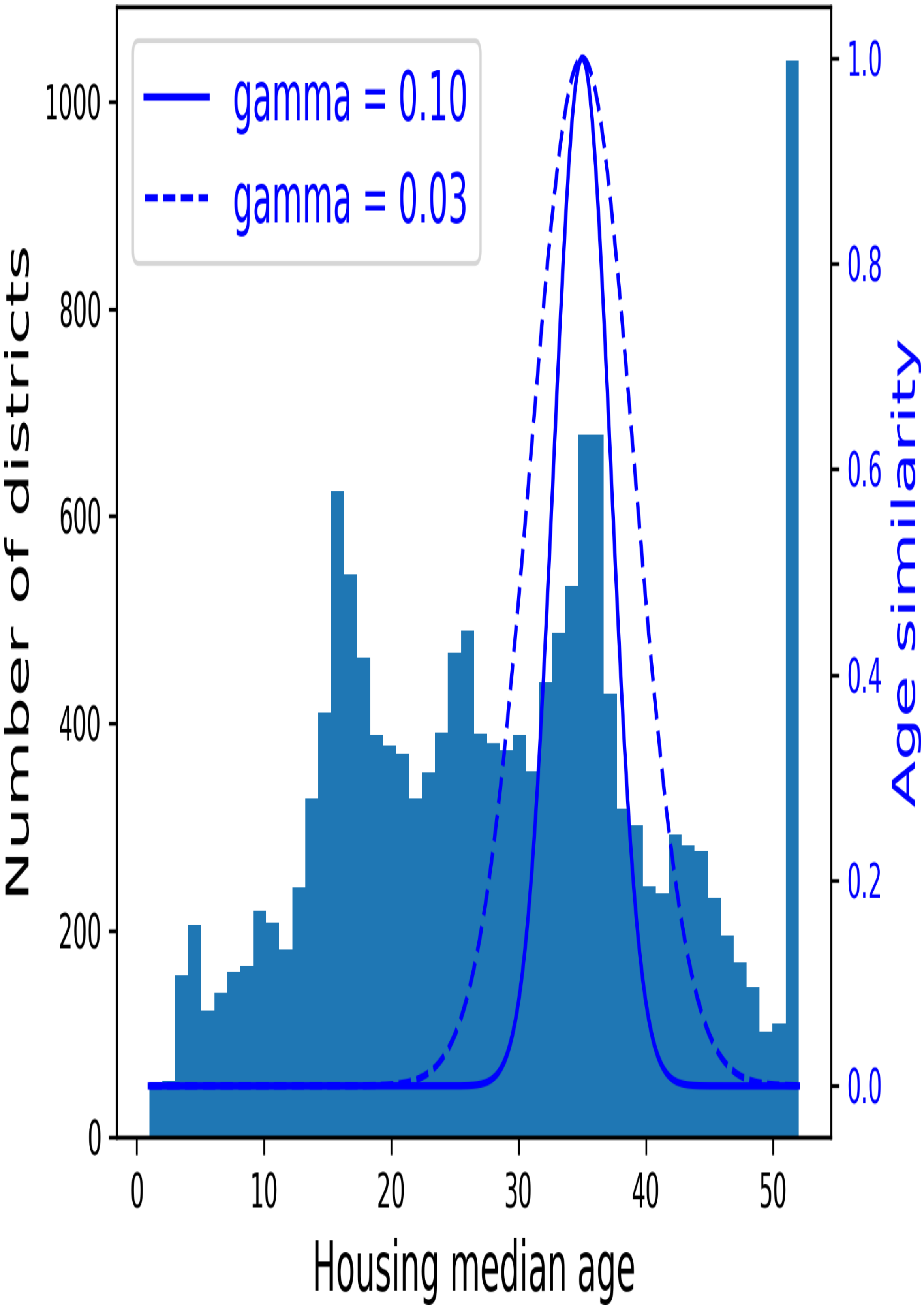


Figure 2-18. Gaussian RBF feature measuring the similarity between the housing median age and 35

So far we've only looked at the input features, but the target values may also need to be transformed. For example, if the target distribution has a heavy tail, you may choose to replace the target with its logarithm. But if you do, the regression model will now predict the *log* of the median house value, not the median house value itself. So you will need to compute the exponential of the model's prediction if you want the predicted median house value.

Luckily, most of Scikit-Learn's transformers have an `inverse_transform()` method, making it easy to compute the inverse of their transformations. For example, the following code example shows how to scale the labels using a `StandardScaler` (just like we did for inputs), then train a simple linear regression model on the resulting scaled labels, and use it to make predictions on some new data, which we transform back to the original scale using the trained scaler's `inverse_transform()` method. Note that we convert the labels from a Pandas Series to a DataFrame, since the `StandardScaler` expects 2D inputs. Also, in this example we just train the model on a single raw input feature (median income), for simplicity.

```
from sklearn.linear_model import LinearRegression

target_scaler = StandardScaler()
scaled_labels =
target_scaler.fit_transform(housing_labels.to_frame())

model = LinearRegression()
model.fit(housing[["median_income"]], scaled_labels)
some_new_data = housing[["median_income"]].iloc[:5]  # pretend this
is new data

scaled_predictions = model.predict(some_new_data)
predictions = target_scaler.inverse_transform(scaled_predictions)
```

This works fine, but there's a simpler way: we can use a `TransformedTargetRegressor`. We just need to construct it, giving it the regression model and the label transformer, then fit it on the training set, using the original unscaled labels. It will automatically use the transformer to scale the labels, and train the regression model on the resulting scaled labels, just like we did above. Then when we make a prediction, it will call the regression model's `predict()` method and use the scaler's `inverse_transform()` method to produce the predictions:

```python
from sklearn.compose import TransformedTargetRegressor

model = TransformedTargetRegressor(LinearRegression(),
                                   transformer=StandardScaler())
model.fit(housing[["median_income"]], housing_labels)
predictions = model.predict(some_new_data)
```

Custom Transformers

Although Scikit-Learn provides many useful transformers, you will need to write your own for tasks such as custom transformations, cleanup operations, or combining specific attributes.

For transformations that don't require any training, you can just write a function that takes a NumPy array as input, and outputs the transformed array. For example, as we discussed in the previous section, it's often a good idea to transform features with heavy-tailed distributions by replacing them with their logarithm (assuming the feature is positive and the tail is on the right). Let's create a log-transformer, and apply it to the population feature:

```python
from sklearn.preprocessing import FunctionTransformer

log_transformer = FunctionTransformer(np.log, inverse_func=np.exp)
log_pop = log_transformer.transform(housing[["population"]])
```

The `inverse_func` argument is optional. It lets you specify an inverse transform function, for example if you plan to use your transformer in a `TransformedTargetRegressor`.

Your transformation function can take hyperparameters as additional arguments. For example, here's how to create a transformer that computes the same Gaussian RBF similarity measure as earlier:

```python
rbf_transformer = FunctionTransformer(rbf_kernel,
                                      kw_args=dict(Y=[[35.]],
gamma=0.1))
age_simil_35 =
rbf_transformer.transform(housing[["housing_median_age"]])
```

Note that there's no inverse function for the RBF kernel, since there are always two values at a given distance from a fixed point (except at distance 0). Also note that rbf_kernel() does not treat the features separately. If you pass it an array with 2 features, it will measure the 2D distance (Euclidean) to measure similarity. For example, here's how to add a feature that will measure the geographic similarity between each district and San Francisco:

```
sf_coords = 37.7749, -122.41
sf_transformer = FunctionTransformer(rbf_kernel,
                                     kw_args=dict(Y=[sf_coords],
gamma=0.1))
sf_simil = sf_transformer.transform(housing[["latitude",
"longitude"]])
```

Custom transformers are also useful to combine features. For example, here's a FunctionTransformer that computes the ratio between the input features 0 and 1:

```
>>> ratio_transformer = FunctionTransformer(lambda X: X[:, [0]] /
X[:, [1]])
>>> ratio_transformer.transform(np.array([[1., 2.], [3., 4.]]))
array([[0.5 ],
       [0.75]])
```

FunctionTransformer is very handy, but what if you would like your transformer to be trainable, learning some parameters in the fit() method and using them later in the transform() method? For this, you need to write a custom class. Scikit-Learn relies on duck typing, so this class does not have to inherit from any particular base class: all it needs is three methods: fit() (which must return self), transform(), and fit_transform().

You can get fit_transform() for free by simply adding TransformerMixin as a base class: the default implementation will just call fit() then transform(). If you add BaseEstimator as a base class (and avoid using *args and **kargs in your constructor), you will also get two extra methods: get_params() and set_params(). These will be useful for automatic hyperparameter tuning.

For example, here's a custom transformer that acts much like the StandardScaler:

```python
from sklearn.base import BaseEstimator, TransformerMixin
from sklearn.utils.validation import check_array, check_is_fitted

class StandardScalerClone(BaseEstimator, TransformerMixin):
    def __init__(self, with_mean=True):  # no *args or **kwargs!
        self.with_mean = with_mean

    def fit(self, X, y=None):  # y is required even though we don't
use it
        X = check_array(X)  # checks that X is an array with finite
float values
        self.mean_ = X.mean(axis=0)
        self.scale_ = X.std(axis=0)
        self.n_features_in_ = X.shape[1]  # every estimator stores
this in fit()
        return self  # always return self!

    def transform(self, X):
        check_is_fitted(self)  # looks for learned attributes (with
trailing _)
        X = check_array(X)
        assert self.n_features_in_ == X.shape[1]
        if self.with_mean:
            X = X - self.mean_
        return X / self.scale_
```

Here are a few things to note:

- The `sklearn.utils.validation` package contains several functions we can use to validate the inputs. For simplicity, we will skip such tests in the rest of this book, but production code should have them.
- Scikit-Learn pipelines require the `fit()` method to have two arguments `X` and `y`, which is why we need the `y=None` argument even though we don't use `y`.
- All Scikit-Learn estimators set `n_features_in_` in the `fit()` method, and they ensure that the data passed to `transform()` or `predict()` has this number of features.
- The `fit()` method must return `self`.
- This implementation is not 100% complete: all estimators should set `feature_names_in_` in the `fit()` method when they are passed

a DataFrame. Moreover, all transformers should provide a `get_feature_names_out()` method, as well as an `inverse_transform()` method when their transformation can be reversed. See the last exercise at the end of this chapter for more details.

> **TIP**
>
> You can check whether your custom estimator respects Scikit-Learn's API by passing an instance to `check_estimator()` from the `sklearn.utils.estimator_checks` package. For the full API, check out *https://scikit-learn.org/stable/developers/*.

A custom transformer can (and often does) use other estimators in its implementation. For example, below we see a custom transformer that uses a `KMeans` clusterer in the `fit()` method to identify the main clusters in the training data, and then uses `rbf_kernel()` in the `transform()` method to measure how similar each sample is to each cluster center:

```
from sklearn.cluster import KMeans

class ClusterSimilarity(BaseEstimator, TransformerMixin):
    def __init__(self, n_clusters=10, gamma=1.0, random_state=None):
        self.n_clusters = n_clusters
        self.gamma = gamma
        self.random_state = random_state

    def fit(self, X, y=None, sample_weight=None):
        self.kmeans_ = KMeans(self.n_clusters,
random_state=self.random_state)
        self.kmeans_.fit(X, sample_weight=sample_weight)
        return self  # always return self!

    def transform(self, X):
        return rbf_kernel(X, self.kmeans_.cluster_centers_,
gamma=self.gamma)

    def get_feature_names_out(self, names=None):
        return [f"Cluster {i} similarity" for i in
range(self.n_clusters)]
```

As we will see in Chapter 9, K-Means is a clustering algorithm that locates clusters in the data. How many it searches for is controlled by the `n_clusters` hyperparameter. After training, the cluster centers are available via the `cluster_centers_` attribute. The `fit()` method of `KMeans` supports an optional argument `sample_weight` which lets the user specify the relative weights of the samples. K-Means is a stochastic algorithm, meaning that it relies on randomness to locate the clusters, so if you want reproducible results, you must set the `random_state` parameter. As you can see, despite the complexity of the task, the code is fairly straightforward. Now let's use this custom transformer:

```
cluster_simil = ClusterSimilarity(n_clusters=10, gamma=1.,
random_state=42)
similarities = cluster_simil.fit_transform(housing[["latitude",
"longitude"]],

sample_weight=housing_labels)
```

This code creates a `ClusterSimilarity` transformer, setting the number of clusters to 10 clusters. Then it calls `fit_transform()` with the latitude and longitude of every district in the training set, weighting each district by its median house value. The transformer uses K-Means to locate the clusters, then measures the Gaussian RBF similarity between each district and all 10 cluster centers. The result is a matrix with one row per district, and one column per cluster. Let's look at the first 3 rows, rounding to 2 decimals:

```
>>> similarities[:3].round(2)
array([[0.  , 0.14, 0.  , 0.  , 0.  , 0.08, 0.  , 0.99, 0.  , 0.6 ],
       [0.63, 0.  , 0.99, 0.  , 0.  , 0.  , 0.04, 0.  , 0.11, 0.  ],
       [0.  , 0.29, 0.  , 0.  , 0.01, 0.44, 0.  , 0.7 , 0.  , 0.3 ]])
```

Figure 2-19 shows the 10 cluster centers found by K-Means. The districts are colored according to their geographic similarity to their closest cluster center. As you can see, most clusters are located in highly populated and expensive areas.

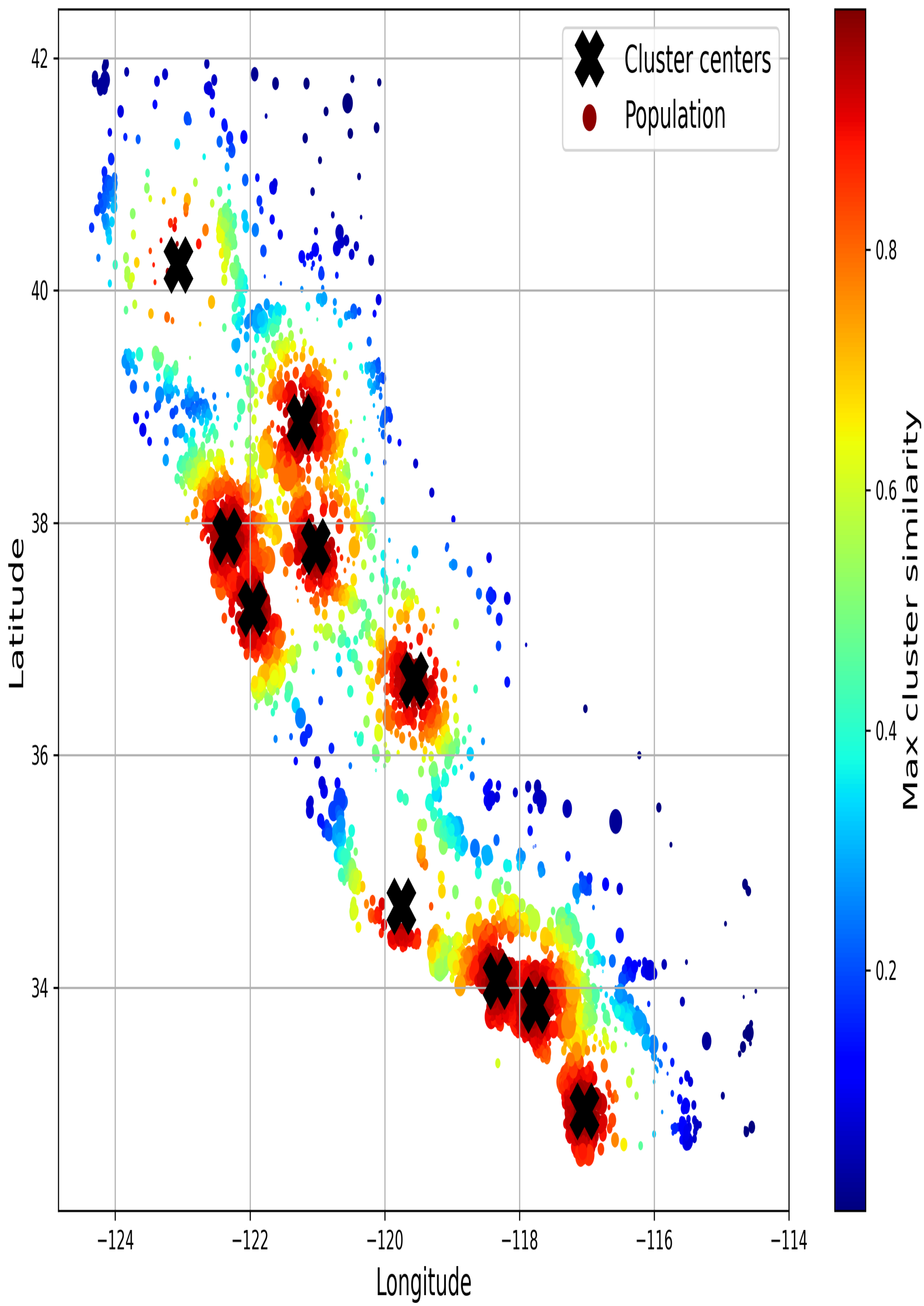


Figure 2-19. Gaussian RBF similarity to the nearest cluster center

Transformation Pipelines

As you can see, there are many data transformation steps that need to be executed in the right order. Fortunately, Scikit-Learn provides the `Pipeline` class to help with such sequences of transformations. Here is a small pipeline for numerical attributes, which will first impute then scale the input features:

```
from sklearn.pipeline import Pipeline

num_pipeline = Pipeline([
    ("impute", SimpleImputer(strategy="median")),
    ("standardize", StandardScaler()),
])
```

The `Pipeline` constructor takes a list of name/estimator pairs (2-tuples) defining a sequence of steps. The names can be anything you like, as long as they are unique and don't contain double underscores, __. They will be useful later when we discuss hyperparameter tuning. The estimators must all be transformers (i.e., they must have a `fit_transform()` method), except for the last one, which can be anything: a transformer, a predictor, or any other type of estimator.

> **TIP**
>
> In a Jupyter notebook, if you `import sklearn` and run `sklearn.set_config(display="diagram")`, all Scikit-Learn estimators will be rendered as interactive diagrams. This is particularly useful to visual pipelines. To visualize `num_pipeline`, run a cell with `num_pipeline` as the last line. Clicking on an estimator will show more details.

If you don't want to bother naming the transformers, you can use the `make_pipeline()` function instead: it just takes a list of transformers as positional arguments, and it creates a `Pipeline` using the names of the transformers' classes, in lower case and without underscores (e.g., "simpleimputer"). In case multiple transformers have the same name, an index is appended to their names (e.g., "foo-1", "foo-2", etc.).

```
from sklearn.pipeline import make_pipeline

num_pipeline = make_pipeline(SimpleImputer(strategy="median"),
StandardScaler())
```

When you call the pipeline's `fit()` method, it calls `fit_transform()` sequentially on all transformers, passing the output of each call as the parameter to the next call until it reaches the final estimator, for which it just calls the `fit()` method.

The pipeline exposes the same methods as the final estimator. In this example, the last estimator is a `StandardScaler` which is a transformer so the pipeline also acts like a transformer. If you call the pipeline's `transform()` method, it will sequentially apply all the transformations to the data. If the last estimator were a predictor instead of a transformer, then the pipeline would have a `predict()` method rather than a `transform()` method. Calling it would sequentially apply all the transformations to the data and pass the result to the predictor's `predict()` method.

Let's call the pipeline's `fit_transform()` method and look at the output's first two rows, rounded to 2 decimals:

```
>>> housing_num_prepared = num_pipeline.fit_transform(housing_num)
>>> housing_num_prepared[:2].round(2)
array([[-1.42,  1.01,  1.86,  0.31,  1.37,  0.14,  1.39, -0.94],
       [ 0.6 , -0.7 ,  0.91, -0.31, -0.44, -0.69, -0.37,  1.17]])
```

As we saw earlier, we can recover a nice DataFrame using the pipeline's `get_feature_names_out()` method:

```
df_housing_num_prepared = pd.DataFrame(
    housing_num_prepared,
columns=num_pipeline.get_feature_names_out(),
    index=housing_num.index)
```

Pipelines support indexing, for example `pipeline[1]` returns the second estimator in the pipeline, and `pipeline[:-1]` returns a `Pipeline` object containing all but the last estimator. You can also access the estimators via the `steps` attribute, which is a list of name/estimator pairs, or via the `name_steps` dictionary attribute which maps the names to the estimators. For example `num_pipeline["simpleimputer"]` returns the estimator named `"simpleimputer"`.

So far, we have handled the categorical columns and the numerical columns separately. It would be more convenient to have a single transformer capable of handling all columns, applying the appropriate transformations to each column. For this, you can use a `ColumnTransformer`. For example, the following `ColumnTransformer` will apply `num_pipeline` (the one we just defined) to the numerical attributes, and `cat_pipeline` to the categorical attribute:

```
from sklearn.compose import ColumnTransformer

num_attribs = ["longitude", "latitude", "housing_median_age",
"total_rooms",
               "total_bedrooms", "population", "households",
"median_income"]
cat_attribs = ["ocean_proximity"]

cat_pipeline = make_pipeline(
    SimpleImputer(strategy="most_frequent"),
    OneHotEncoder(handle_unknown="ignore"))

preprocessing = ColumnTransformer([
    ("num", num_pipeline, num_attribs),
    ("cat", cat_pipeline, cat_attribs),
])
```

First we import the `ColumnTransformer` class, next we define the list of numerical and categorical column names, we construct a simple pipeline for categorical attributes, and lastly we construct a `ColumnTransformer`. Its constructor requires a list of triplets (3-tuples), each containing a name (which must be unique and not contain double underscores), a transformer, and a list of names (or indices) of columns that the transformer should be applied to.

TIP

Instead of using a transformer, you can specify the string "drop" if you want the columns to be dropped, or you can specify "passthrough" if you want the columns to be left untouched. By default, the remaining columns (i.e., the ones that were not listed) will be dropped, but you can set the remainder hyperparameter to any transformer (or to "passthrough") if you want these columns to be handled differently.

Since listing all the column names is not very convenient, Scikit-Learn provides a make_column_selector() function that returns a selector function you can use to automatically select all the features of a given type, such as numerical or categorical. This selector function can be passed to the ColumnTransformer instead of column names or indices. Moreover, if you don't care about naming the transformers, you can use make_column_transformer() which chooses the names for you, just like make_pipeline() does. For example, the following code creates the same ColumnTransformer as above, except the transformers are automatically named "pipeline-1" and "pipeline-2" instead of "num" and "cat":

```
from sklearn.compose import make_column_selector,
make_column_transformer

preprocessing = make_column_transformer(
    (num_pipeline, make_column_selector(dtype_include=np.number)),
    (cat_pipeline, make_column_selector(dtype_include=np.object)),
)
```

Now we're ready to apply this ColumnTransformer to the housing data:

```
housing_prepared = preprocessing.fit_transform(housing)
```

Great! We have a preprocessing pipeline that takes the entire training data and applies each transformer to the appropriate columns, then concatenates the transformed columns horizontally (transformers must never change the number of rows). Once again this returns a NumPy array, but you can get the column names using preprocessing.get_feature_names_out() and wrap the data in a nice DataFrame as we did before.

NOTE

The `OneHotEncoder` returns a sparse matrix, while the `num_pipeline` returns a dense matrix. When there is such a mix of sparse and dense matrices, the `ColumnTransformer` estimates the density of the final matrix (i.e., the ratio of nonzero cells), and it returns a sparse matrix if the density is lower than a given threshold (by default, `sparse_threshold=0.3`). In this example, it returns a dense matrix.

Your project's going really well, you're almost ready to train some models! You now want to create a single pipeline that will perform all the transformations you've experimented with up to now. Let's recap what the pipeline will do and why:

- Missing values in numerical features will be imputed by replacing them with the median, as most ML algorithms don't expect missing values. As for the categorical feature, any missing values will be replaced by the most frequent category.
- The categorical feature will be one-hot encoded, as most ML algorithms only accept numerical inputs.
- A few ratio features will be computed and added: `bedrooms_ratio`, `rooms_per_house` and `people_per_house`. Hopefully these will better correlate with the median housing value, and thereby help the ML models.
- A few cluster similarity features will also be added. These will likely be more useful to the model than latitude and longitude.
- Features with a long tail will be replaced by their logarithm, as most models prefer features with roughly uniform or Gaussian distributions.
- All numerical features will be standardized, as most ML algorithms prefer when all features have roughly the same scale.

The code that builds the pipeline to do all of this has no secret for you by now:

```
def column_ratio(X):
    return X[:, [0]] / X[:, [1]]
```

```
def ratio_pipeline(name=None):
    return make_pipeline(
        SimpleImputer(strategy="median"),
        FunctionTransformer(column_ratio,
                            feature_names_out=lambda input_features:
[name]),
        StandardScaler())

log_pipeline = make_pipeline(SimpleImputer(strategy="median"),
                             FunctionTransformer(np.log),
                             StandardScaler())
cluster_simil = ClusterSimilarity(n_clusters=10, gamma=1.,
random_state=42)
default_num_pipeline =
make_pipeline(SimpleImputer(strategy="median"),
                                     StandardScaler())
preprocessing = ColumnTransformer([
        ("bedrooms_ratio", ratio_pipeline("bedrooms_ratio"),
                           ["total_bedrooms", "total_rooms"]),
        ("rooms_per_house", ratio_pipeline("rooms_per_house"),
                            ["total_rooms", "households"]),
        ("people_per_house", ratio_pipeline("people_per_house"),
                             ["population", "households"]),
        ("log", log_pipeline, ["total_bedrooms", "total_rooms",
                               "population", "households",
"median_income"]),
        ("geo", cluster_simil, ["latitude", "longitude"]),
        ("cat", cat_pipeline,
make_column_selector(dtype_include=np.object)),
    ],
    remainder=default_num_pipeline)  # one column remaining:
housing_median_age
```

If you run this column transformer, it performs all the transformations and outputs a NumPy array with 24 features:

```
>>> housing_prepared = preprocessing.fit_transform(housing)
>>> housing_prepared.shape
(16512, 24)
>>> preprocessing.get_feature_names_out()
array(['bedrooms_ratio__bedrooms_ratio',
       'rooms_per_house__rooms_per_house',
       'people_per_house__people_per_house', 'log__total_bedrooms',
       'log__total_rooms', 'log__population', 'log__households',
       'log__median_income', 'geo__Cluster 0 similarity', [...],
       'geo__Cluster 9 similarity', 'cat__ocean_proximity_<1H OCEAN',
       'cat__ocean_proximity_INLAND', 'cat__ocean_proximity_ISLAND',
       'cat__ocean_proximity_NEAR BAY', 'cat__ocean_proximity_NEAR
```

```
OCEAN',
       'remainder__housing_median_age'], dtype=object)
```

Select and Train a Model

At last! You framed the problem, you got the data and explored it, you sampled a training set and a test set, and you wrote a preprocessing pipeline to automatically clean up and prepare your data for Machine Learning algorithms. You are now ready to select and train a Machine Learning model.

Training and Evaluating on the Training Set

The good news is that thanks to all these previous steps, things are now going to be easy! You decide to train a very basic Linear Regression model to get started:

```
from sklearn.linear_model import LinearRegression

lin_reg = make_pipeline(preprocessing, LinearRegression())
lin_reg.fit(housing, housing_labels)
```

Done! You now have a working Linear Regression model. Let's try it out on the training set, looking at the first 5 predictions and comparing them to the labels:

```
>>> housing_predictions = lin_reg.predict(housing)
>>> housing_predictions[:5].round(-2)  # -2 = rounded to the nearest
hundred
array([243700., 372400., 128800.,  94400., 328300.])
>>> housing_labels.iloc[:5].values
array([458300., 483800., 101700.,  96100., 361800.])
```

Well, it works, but not always: the first prediction is way off (by over $200,000!), while the other predictions are better: two are off by about 25%, and two are off by less than 10%. Remember that you chose to use the RMSE as your performance measure, so you want to measure this regression model's RMSE on the whole training set using Scikit-Learn's `mean_squared_error()` function, with the `squared` argument set to `False`:

```
>>> from sklearn.metrics import mean_squared_error
>>> lin_rmse = mean_squared_error(housing_labels,
housing_predictions,
...                               squared=False)
...
>>> lin_rmse
68687.89176589991
```

This is better than nothing, but clearly not a great score: most districts' `median_housing_values` range between $120,000 and $265,000, so a typical prediction error of $68,628 is really not very satisfying. This is an example of a model underfitting the training data. When this happens it can mean that the features do not provide enough information to make good predictions, or that the model is not powerful enough. As we saw in the previous chapter, the main ways to fix underfitting are to select a more powerful model, to feed the training algorithm with better features, or to reduce the constraints on the model. This model is not regularized, which rules out the last option. You could try to add more features, but first you want to try a more complex model to see how it does.

So you decide to try a `DecisionTreeRegressor`, as this is a fairly powerful model capable of finding complex nonlinear relationships in the data (Decision Trees are presented in more detail in Chapter 6):

```
from sklearn.tree import DecisionTreeRegressor

tree_reg = make_pipeline(preprocessing,
DecisionTreeRegressor(random_state=42))
tree_reg.fit(housing, housing_labels)
```

Now that the model is trained, you evaluate it on the training set:

```
>>> housing_predictions = tree_reg.predict(housing)
>>> tree_rmse = mean_squared_error(housing_labels,
housing_predictions,
...                               squared=False)
...
>>> tree_rmse
0.0
```

Wait, what!? No error at all? Could this model really be absolutely perfect? Of course, it is much more likely that the model has badly overfit the data. How can you be sure? As we saw earlier, you don't want to touch the test set until you are ready to launch a model you are confident about, so you need to use part of the training set for training and part of it for model validation.

Better Evaluation Using Cross-Validation

One way to evaluate the Decision Tree model would be to use the `train_test_split()` function to split the training set into a smaller training set and a validation set, then train your models against the smaller training set and evaluate them against the validation set. It's a bit of work, but nothing too difficult, and it would work fairly well.

A great alternative is to use Scikit-Learn's *K-fold cross-validation* feature. The following code randomly splits the training set into 10 non-overlapping subsets called *folds*, then it trains and evaluates the Decision Tree model 10 times, picking a different fold for evaluation every time and using the other 9 folds for training. The result is an array containing the 10 evaluation scores:

```
from sklearn.model_selection import cross_val_score

tree_rmses = -cross_val_score(tree_reg, housing, housing_labels,
                              scoring="neg_root_mean_squared_error",
cv=10)
```

> **WARNING**
>
> Scikit-Learn's cross-validation features expect a utility function (greater is better) rather than a cost function (lower is better), so the scoring function is actually the opposite of the RMSE. It's a negative value, which is why we need to switch the sign of the output to get the RMSE scores.

Let's look at the results:

```
>>> pd.Series(tree_rmses).describe()
count       10.000000
mean     66868.027288
std       2060.966425
min      63649.536493
25%      65338.078316
50%      66801.953094
```

```
75%      68229.934454
max      70094.778246
dtype: float64
```

Now the Decision Tree doesn't look as good as it did earlier. In fact, it seems to perform almost as poorly as the Linear Regression model! Notice that cross-validation allows you to get not only an estimate of the performance of your model, but also a measure of how precise this estimate is (i.e., its standard deviation). The Decision Tree has an RMSE of about 66,868, with a standard deviation of about 2,061. You would not have this information if you just used one validation set. But cross-validation comes at the cost of training the model several times, so it is not always feasible.

If you compute the same metric for the Linear Regression model, you will find that the mean RMSE is 69,858 and the standard deviation is 4,182. So the Decision Tree model seems to perform very slightly better than the linear model, but only marginally better due to severe overfitting. We know there's an overfitting problem because the training error is low (actually zero) while the validation error is high.

Let's try one last model now: the `RandomForestRegressor`. As we will see in Chapter 7, Random Forests work by training many Decision Trees on random subsets of the features, then averaging out their predictions. Such models composed of many other models are called *ensembles*: they are capable of boosting the performance of the underlying model (in this case, Decision Trees). The code is much the same as earlier:

```
from sklearn.ensemble import RandomForestRegressor

forest_reg = make_pipeline(preprocessing,
                           RandomForestRegressor(random_state=42))
forest_rmses = -cross_val_score(forest_reg, housing, housing_labels,

scoring="neg_root_mean_squared_error", cv=10)
```

Let's look at these scores:

```
>>> pd.Series(forest_rmses).describe()
count       10.000000
mean     47019.561281
std       1033.957120
```

```
min      45458.112527
25%      46464.031184
50%      46967.596354
75%      47325.694987
max      49243.765795
dtype: float64
```

Wow, this is much better: Random Forests really look very promising for this task! However, if you train a `RandomForest` and measure the RMSE on the training set, you will find about 17,474: that's much lower, meaning that there's still quite a lot of overfitting going on. Possible solutions are to simplify the model, constrain it (i.e., regularize it), or get a lot more training data. Before you dive much deeper into Random Forests, however, you should try out many other models from various categories of Machine Learning algorithms (e.g., several Support Vector Machines with different kernels, and possibly a neural network), without spending too much time tweaking the hyperparameters. The goal is to shortlist a few (two to five) promising models.

Fine-Tune Your Model

Let's assume that you now have a shortlist of promising models. You now need to fine-tune them. Let's look at a few ways you can do that.

Grid Search

One option would be to fiddle with the hyperparameters manually, until you find a great combination of hyperparameter values. This would be very tedious work, and you may not have time to explore many combinations.

Instead, you can use Scikit-Learn's `GridSearchCV` class to search for you. All you need to do is tell it which hyperparameters you want it to experiment with and what values to try out, and it will use cross-validation to evaluate all the possible combinations of hyperparameter values. For example, the following code searches for the best combination of hyperparameter values for the `RandomForestRegressor`:

```
from sklearn.model_selection import GridSearchCV

full_pipeline = Pipeline([
```

```
    ("preprocessing", preprocessing),
    ("random_forest", RandomForestRegressor(random_state=42)),
])
param_grid = [
    {'preprocessing__geo__n_clusters': [5, 8, 10],
     'random_forest__max_features': [4, 6, 8]},
    {'preprocessing__geo__n_clusters': [10, 15],
     'random_forest__max_features': [6, 8, 10]},
]
grid_search = GridSearchCV(full_pipeline, param_grid, cv=3,
                           scoring='neg_root_mean_squared_error')
grid_search.fit(housing, housing_labels)
```

Notice that you can refer to any hyperparameter of any estimator in a pipeline, even if this estimator is nested deep inside several pipelines and column transformers. For example, when Scikit-Learn sees `"preprocessing__geo__n_clusters"`, it splits this string at the double underscores, then it looks for an estimator named `"preprocessing"` inside the pipeline and finds the preprocessing `ColumnTransformer`. Then it looks for a transformer named `"geo"` inside this `ColumnTransformer` and finds the `ClusterSimilarity` transformer we used on the latitude and longitude attributes. The it finds this transformer's `n_clusters` hyperparameter. Similarly, `random_forest__max_features` refers to the `max_features` hyperparameter of the estimator named "random_forest", which is of course the `RandomForest` model (the `max_features` hyperparameter will be explained in Chapter 7).

> **TIP**
>
> Wrapping preprocessing steps in a Scikit-Learn pipeline allows you to tune the preprocessing hyperparameters along with the model hyperparameters. This is a good thing since they often interact. For example, perhaps increasing `n_clusters` requires increasing `max_features` as well. If fitting the pipeline transformers is computationally expensive, you can set the pipeline's `memory` hyperparameter to the path of a caching directory: when you first fit the pipeline, Scikit-Learn will save the fitted transformers to this directory. If you then fit the pipeline again with the same hyperparameters, Scikit-Learn will just load the cached transformers.

There are two dictionaries in this `param_grid`, so `GridSearchCV` will first evaluate all 3 × 3 = 9 combinations of `n_clusters` and `max_features` hyperparameter values specified in the first `dict`, then it will try all 2 × 3 = 6 combinations of hyperparameter values in the second `dict`. So in total the grid search will explore 9 + 6 = 15 combinations of hyperparameter values, and it will train the pipeline 3 times per combination, since we are using three-fold cross validation. So there will be a grand total of 15 × 3 = 45 rounds of training! It may take a while, but when it is done you can get the best combination of parameters like this:

```
>>> grid_search.best_params_
{'preprocessing__geo__n_clusters': 15, 'random_forest__max_features':
6}
```

In this example, the best model is obtained by setting `n_clusters` to 15 and `max_features` to 8.

> **TIP**
>
> Since 15 is the maximum value that was evaluated for `n_clusters`, you should probably try searching again with higher values; the score may continue to improve.

The best estimator is available using `grid_search.best_estimator_`. If `GridSearchCV` is initialized with `refit=True` (which is the default), then once it finds the best estimator using cross-validation, it retrains it on the whole training set. This is usually a good idea, since feeding it more data will likely improve its performance.

The evaluation scores are available using `grid_search.cv_results_`. This is a dictionary, but if you wrap it in a DataFrame, you get a nice list of all the test scores for each combination of hyperparameters and for each cross-validation split, as well as the mean test score across all splits.

```
>>> cv_res = pd.DataFrame(grid_search.cv_results_)
>>> cv_res.sort_values(by="mean_test_score", ascending=False,
inplace=True)
>>> [...]  # change column names to fit on this page, and show rmse =
-score
>>> cv_res.head()
   n_clusters max_features  split0  split1  split2  mean_test_rmse
12         15            6   43460   43919   44748           44042
```

```
13          15            8   44132   44075   45010             44406
14          15           10   44374   44286   45316             44659
7           10            6   44683   44655   45657             44999
9           10            6   44683   44655   45657             44999
```

The mean test RMSE score for the best model is 44,042, which is better than the score you got earlier using the default hyperparameter values (which was 47,019). Congratulations, you have successfully fine-tuned your best model!

Randomized Search

The grid search approach is fine when you are exploring relatively few combinations, like in the previous example, but `RandomizedSearchCV` is often preferable, especially when the hyperparameter search space is large. This class can be used in much the same way as the `GridSearchCV` class, but instead of trying out all possible combinations, it evaluates a fixed number of combinations, selecting a random value for each hyperparameter at every iteration. This may sound surprising, but this approach has several benefits:

- If some of your hyperparameters are continuous (or discrete but with many possible values), and you let randomized search run for, say, 1,000 iterations, then it will explore 1,000 different values for each of these hyperparameters, whereas grid search would only explore the few values you listed for each one.
- Suppose a hyperparameter does not actually make much difference, but you don’t know it yet. If it has 10 possible values you add it to your grid search, then training will take 10 times longer. But if you add it to a random search, it will not make any difference.
- Suppose there are 6 hyperparameters to explore, each with 10 possible values, then grid search offers no other choice than training the model a million times, whereas random search can always run for any number of iterations you choose.

For each hyperparameter, you must provide either a list of possible values, or a probability distribution:

```python
from sklearn.model_selection import RandomizedSearchCV
from scipy.stats import randint

param_distribs = {'preprocessing__geo__n_clusters': randint(low=3,
high=50),
                  'random_forest__max_features': randint(low=2,
high=20)}

rnd_search = RandomizedSearchCV(
    full_pipeline, param_distributions=param_distribs, n_iter=10,
cv=3,
    scoring='neg_root_mean_squared_error', random_state=42)

rnd_search.fit(housing, housing_labels)
```

Scikit-Learn also has two other hyperparameter search classes: `HalvingRandomSearchCV` and `HalvingGridSearchCV`. Their goal is to use the computational resources more efficiently, either to train faster or to explore a larger hyperparameter space. Here's how they work: in the first round, many hyperparameter combinations (called "candidates") are generated using either the grid approach or the random approach. These candidates are then used to train models which are then evaluated using cross-validation, as usual. However, training uses limited resources which speeds up this first round considerably. By default, "limited resources" means that the models are trained on a small part of the training set. However, other limitations are possible, such as reducing the number of training iterations if the model has a hyperparameter to set it. Once every candidate has been evaluated, only the best ones go on to the second round, where they are allowed more resources to compete. After several rounds, the final candidates are evaluated using full resources. This may save you some time tuning hyperparameters.

Ensemble Methods

Another way to fine-tune your system is to try to combine the models that perform best. The group (or "ensemble") will often perform better than the best individual model—just like Random Forests perform better than the individual Decision Trees they rely on—especially if the individual models make very different types of errors. For example, you could train and fine-tune a k-Nearest Neighbors model, then create an ensemble model that just predicts the mean of the random forest prediction and the KNN's prediction. We will cover this topic in more detail in Chapter 7.

Analyze the Best Models and Their Errors

You will often gain good insights on the problem by inspecting the best models. For example, the `RandomForestRegressor` can indicate the relative importance of each attribute for making accurate predictions:

```
>>> final_model = rnd_search.best_estimator_  # includes
preprocessing
>>> feature_importances =
final_model["random_forest"].feature_importances_
>>> feature_importances.round(2)
array([0.07, 0.05, 0.05, 0.01, 0.01, 0.01, 0.01, 0.19, [...], 0.01])
```

Let's sort these importance scores in descending order and display them next to their corresponding attribute names:

```
>>> sorted(zip(feature_importances,
...            final_model["preprocessing"].get_feature_names_out()),
...            reverse=True)
...
[(0.18694559869103852, 'log__median_income'),
 (0.0748194905715524, 'cat__ocean_proximity_INLAND'),
 (0.06926417748515576, 'bedrooms_ratio__bedrooms_ratio'),
 (0.05446998753775219, 'rooms_per_house__rooms_per_house'),
 (0.05262301809680712, 'people_per_house__people_per_house'),
 (0.03819415873915732, 'geo__Cluster 0 similarity'),
 [...]
 (0.00015061247730531558, 'cat__ocean_proximity_NEAR BAY'),
 (7.301686597099842e-05, 'cat__ocean_proximity_ISLAND')]
```

With this information, you may want to try dropping some of the less useful features (e.g., apparently only one `ocean_proximity` category is really useful, so you could try dropping the others).

> **TIP**
>
> The `sklearn.feature_selection.SelectFromModel` transformer can automatically drop the least useful features for you: when you fit it, it trains a model (typically a random forest), it looks at its `feature_importances_` attribute, and it selects the most useful features. Then when you call `transform()`, it just drops the other features.

You should also look at the specific errors that your system makes, then try to understand why it makes them and what could fix the problem: adding extra features or getting rid of uninformative ones, cleaning up outliers, etc.

Now is also a good time to ensure that your model not only works well on average, but also on all categories of districts, whether they're rural or urban, rich or poor, North or South, minority or not, etc. This requires a bit of work creating subsets of your validation set for each category, but it's important: if your model performs poorly on a whole category of districts, then it should probably not be deployed until the issue is solved, or at least it should not be used to make predictions for that category, as it may do more harm than good.

Evaluate Your System on the Test Set

After tweaking your models for a while, you eventually have a system that performs sufficiently well. You are ready to evaluate the final model on the test set. There is nothing special about this process; just get the predictors and the labels from your test set, and run your `final_model` to transform the data and make predictions, then evaluate these predictions:

```
X_test = strat_test_set.drop("median_house_value", axis=1)
y_test = strat_test_set["median_house_value"].copy()

final_predictions = final_model.predict(X_test)

final_rmse = mean_squared_error(y_test, final_predictions,
squared=False)
print(final_rmse)   # prints 41424.40026462184
```

In some cases, such a point estimate of the generalization error will not be quite enough to convince you to launch: what if it is just 0.1% better than the model currently in production? You might want to have an idea of how precise this estimate is. For this, you can compute a 95% *confidence interval* for the generalization error using `scipy.stats.t.interval()`. We get a fairly large interval from 39,275 to 43,467, and our previous point estimate of 41,424 is roughly in the middle of it:

```
>>> from scipy import stats
>>> confidence = 0.95
>>> squared_errors = (final_predictions - y_test) ** 2
>>> np.sqrt(stats.t.interval(confidence, len(squared_errors) - 1,
...                          loc=squared_errors.mean(),
...                          scale=stats.sem(squared_errors)))
...
array([39275.40861216, 43467.27680583])
```

If you did a lot of hyperparameter tuning, the performance will usually be slightly worse than what you measured using cross-validation. That's because your system ends up fine-tuned to perform well on the validation data and will likely not perform as well on unknown datasets. It is not the case in this example since the test RMSE is lower than the validation RMSE, but when it happens you must resist the temptation to tweak the hyperparameters to make the numbers look good on the test set; the improvements would be unlikely to generalize to new data.

Now comes the project prelaunch phase: you need to present your solution (highlighting what you have learned, what worked and what did not, what assumptions were made, and what your system's limitations are), document everything, and create nice presentations with clear visualizations and easy-to-remember statements (e.g., "the median income is the number one predictor of housing prices"). In this California housing example, the final performance of the system is not much better than the experts' price estimates which were often off by 30%, but it may still be a good idea to launch it, especially if this frees up some time for the experts so they can work on more interesting and productive tasks.

Launch, Monitor, and Maintain Your System

Perfect, you got approval to launch! You now need to get your solution ready for production (e.g., polish the code, write documentation and tests, and so on). Then you can deploy your model to your production environment. The most basic way to do this is just to save the best model you trained, transfer the file to your production environment, and load it. To save the model, you can use the `joblib` library like this:

```
import joblib

joblib.dump(final_model, "my_california_housing_model.pkl")
```

> **TIP**
>
> It's often a good idea to save every model you experiment with so that you can come back easily to any model you want. You may also save the cross-validation scores and perhaps the actual predictions on the validation set. This will allow you to easily compare scores across model types, and compare the types of errors they make.

Once your model is transferred to production, you can load it and use it. For this you must first import any custom classes and functions the model relies on (which means transferring the code to production), then load the model using `joblib` and use it to make predictions:

```
import joblib
[...]  # import KMeans, BaseEstimator, TransformerMixin, rbf_kernel,
etc.

def column_ratio(X):
    return X[:, [0]] / X[:, [1]]

class ClusterSimilarity(BaseEstimator, TransformerMixin):
    [...]

final_model_reloaded = joblib.load("my_california_housing_model.pkl")

new_data = [...]  # some new districts to make predictions for
predictions = final_model_reloaded.predict(new_data)
```

For example, perhaps the model will be used within a website: the user will type in some data about a new district and click the "Estimate Price" button. This will send a query containing the data to the web server, which will forward it to your web application, and finally your code will simply call the model's `predict()` method (you want to load the model upon server startup, rather than every time the model is used). Alternatively, you can wrap the model within a dedicated web service that your web application can query through a REST API[13] (see Figure 2-20). This makes it easier to upgrade your model to new versions without interrupting the main application. It also simplifies scaling, since you can start as many web services as needed and load-balance the requests coming from your web application across these web services. Moreover, it allows your web application to use any programming language, not just Python.

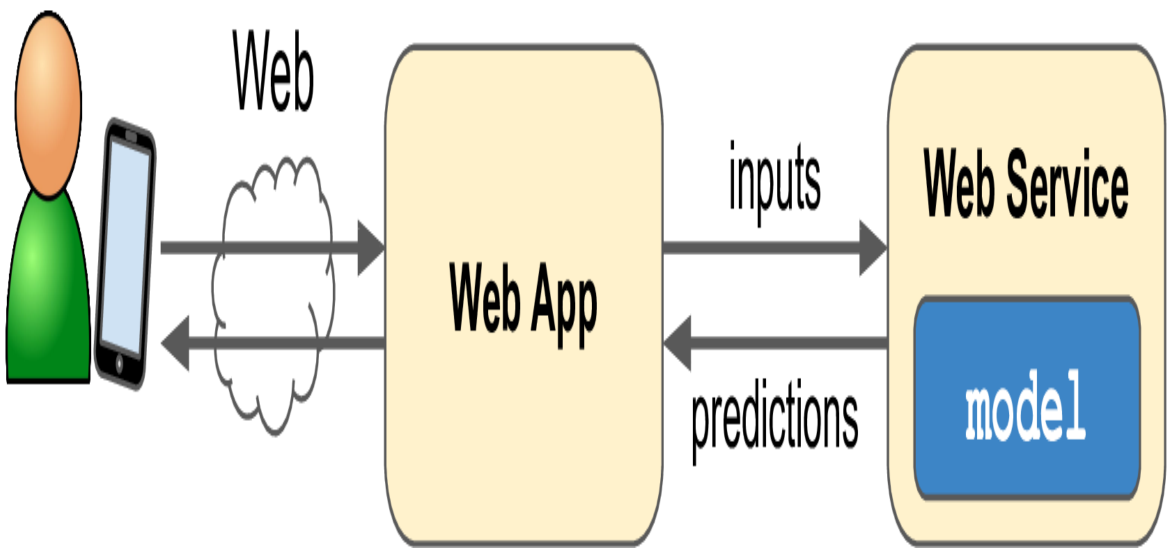


Figure 2-20. A model deployed as a web service and used by a web application

Another popular strategy is to deploy your model to the cloud, for example on Google's Vertex AI (formerly known as Google Cloud AI Platform and Google Cloud ML Engine): just save your model using `joblib` and upload it to Google Cloud Storage (GCS), then head over to Google Cloud AI Platform and create a new model version, pointing it to the GCS file. That's it! This gives you a simple web service that takes care of load balancing and scaling for you. It takes JSON requests containing the input data (e.g., of a district) and returns JSON responses containing the predictions. You can then use this web service in your website (or whatever production environment you are using). As we will see in Chapter 19, deploying TensorFlow models on Vertex AI is not much different from deploying Scikit-Learn models.

But deployment is not the end of the story. You also need to write monitoring code to check your system's live performance at regular intervals and trigger alerts when it drops. It may drop very quickly, for example if a component breaks in your infrastructure, but be aware that it could also decay very slowly, which can easily go unnoticed for a long time. This is quite common because of model rot: if the model was trained with last year's data, it may not be adapted to today's data.

So you need to monitor your model's live performance. But how do you that? Well, it depends. In some cases, the model's performance can be inferred from downstream metrics. For example, if your model is part of a recommender system and it suggests products that the users may be interested in, then it's easy to monitor the number of recommended products sold each day. If this number drops (compared to non-recommended products), then the prime suspect is the model. This may be because the data pipeline is broken, or perhaps the model needs to be retrained on fresh data (as we will discuss shortly).

However, you may also need human analysis to determine the model's performance. For example, suppose you trained an image classification model (which we will see in Chapter 3) to detect several product defects on a production line. How can you get an alert if the model's performance drops, before thousands of defective products get shipped to your clients? One solution is to send to human raters a sample of all the pictures that the model classified (especially pictures that the model wasn't so sure about). Depending on the task, the raters may need to be experts, or they could be nonspecialists, such as workers on a crowdsourcing platform (e.g., Amazon Mechanical Turk). In some applications they could even be the users themselves, responding for example via surveys or repurposed captchas.[14]

Either way, you need to put in place a monitoring system (with or without human raters to evaluate the live model), as well as all the relevant processes to define what to do in case of failures and how to prepare for them. Unfortunately, this can be a lot of work. In fact, it is often much more work than building and training a model.

If the data keeps evolving, you will need to update your datasets and retrain your model regularly. You should probably automate the whole process as much as possible. Here are a few things you can automate:

- Collect fresh data regularly and label it (e.g., using human raters).
- Write a script to train the model and fine-tune the hyperparameters automatically. This script could run automatically, for example every day or every week, depending on your needs.
- Write another script that will evaluate both the new model and the previous model on the updated test set, and deploy the model to production if the performance has not decreased (if it did, make sure you investigate why). The script should probably test the performance of your model on various subsets of the test set, such as poor or rich districts, rural or urban districts, etc.

You should also make sure you evaluate the model's input data quality. Sometimes performance will degrade slightly because of a poor-quality signal (e.g., a malfunctioning sensor sending random values, or another team's output becoming stale), but it may take a while before your system's performance degrades enough to trigger an alert. If you monitor your model's inputs, you may catch this earlier. For example, you could trigger an alert if more and more inputs are missing a feature, or if its mean or standard deviation drifts too far from the training set, or a categorical feature starts containing new categories.

Finally, make sure you keep backups of every model you create and have the process and tools in place to roll back to a previous model quickly, in case the new model starts failing badly for some reason. Having backups also makes it possible to easily compare new models with previous ones. Similarly, you should keep backups of every version of your datasets so that you can roll back to a previous dataset if the new one ever gets corrupted (e.g., if the fresh data that gets added to it turns out to be full of outliers). Having backups of your datasets also allows you to evaluate any model against any previous dataset.

As you can see, Machine Learning involves quite a lot of infrastructure. Chapter 19 discusses some aspects of this, but it's a very broad topic called *ML Operations* (ML Ops) which deserves its own book. So don't be surprised if your first ML project takes a lot of effort and time to build and deploy to production. Fortunately, once all the infrastructure is in place, going from idea to production will be much faster.

Try It Out!

Hopefully this chapter gave you a good idea of what a Machine Learning project looks like as well as showing you some of the tools you can use to train a great system. As you can see, much of the work is in the data preparation step: building monitoring tools, setting up human evaluation pipelines, and automating regular model training. The Machine Learning algorithms are important, of course, but it is probably preferable to be comfortable with the overall process and know three or four algorithms well rather than to spend all your time exploring advanced algorithms.

So, if you have not already done so, now is a good time to pick up a laptop, select a dataset that you are interested in, and try to go through the whole process from A to Z. A good place to start is on a competition website such as *http://kaggle.com/*: you will have a dataset to play with, a clear goal, and people to share the experience with. Have fun!

Exercises

The following exercises are based on this chapter's housing dataset:

1. Try a Support Vector Machine regressor (`sklearn.svm.SVR`) with various hyperparameters, such as `kernel="linear"` (with various values for the `C` hyperparameter) or `kernel="rbf"` (with various values for the `C` and `gamma` hyperparameters). Note that SVMs don't scale well to large datasets, so you should probably train your model on just the first 5,000 instances of the training set and use only 3-fold cross-validation, or else it will take hours. Don't worry about what the hyperparameters mean for now, we'll discuss them in Chapter 5. How does the best `SVR` predictor perform?

2. Try replacing the `GridSearchCV` with a `RandomizedSearchCV`.

3. Try adding a `SelectFromModel` transformer in the preparation pipeline to select only the most important attributes.

4. Try creating a custom transformer that trains a k-Nearest Neighbors regressor (`sklearn.neighbors.KNeighborsRegressor`) in

its `fit()` method, and outputs the model's predictions in its `transform()` method. Then add this feature to the preprocessing pipeline, using latitude and longitude as the inputs to this transformer. This will add a feature in the model that corresponds to the housing median price of the nearest districts.

5. Automatically explore some preparation options using `GridSearchCV`.

6. Try to implement the `StandardScalerClone` class again from scratch, then add support for the `inverse_transform()` method: executing `scaler.inverse_transform(scaler.fit_transform(X))` should return an array very close to `X`. Then add support for feature names: set `feature_names_in_` in the `fit()` method if the input is a DataFrame. This attribute should be a NumPy array of column names. Lastly, implement the `get_feature_names_out()` method: it should have one optional `input_features=None` argument. If passed, the method should check that its length matches `n_features_in_`, and it should match `feature_names_in_` if it is defined, then `input_features` should be returned. If `input_features` is `None`, then the method should return `feature_names_in_` if it is defined or `np.array(["x0", "x1", ...])` with length `n_features_in_` otherwise.

Solutions to these exercises are available at the end of this chapter's notebook, at *https://homl.info/colab3*.

---

1 The original dataset appeared in R. Kelley Pace and Ronald Barry, "Sparse Spatial Autoregressions," *Statistics & Probability Letters* 33, no. 3 (1997): 291–297.

2 A piece of information fed to a Machine Learning system is often called a *signal*, in reference to Claude Shannon's information theory, which he developed at Bell Labs to improve telecommunications. His theory: you want a high signal-to-noise ratio.

3 Recall that the transpose operator flips a column vector into a row vector (and vice versa).

4 You might also need to check legal constraints, such as private fields that should never be copied to unsafe data stores.

5 The standard deviation is generally denoted σ (the Greek letter sigma), and it is the square root of the *variance*, which is the average of the squared deviation from the mean. When a feature has a bell-shaped *normal distribution* (also called a *Gaussian distribution*), which is very common, the “68-95-99.7” rule applies: about 68% of the values fall within 1σ of the mean, 95% within 2σ, and 99.7% within 3σ.

6 You will often see people set the random seed to 42. This number has no special property, other than to be the Answer to the Ultimate Question of Life, the Universe, and Everything.

7 The location information is actually quite coarse, and as a result many districts will have the exact same ID, so they will end up in the same set (test or train). This introduces some unfortunate sampling bias.

8 If you are reading this in grayscale, grab a red pen and scribble over most of the coastline from the Bay Area down to San Diego (as you might expect). You can add a patch of yellow around Sacramento as well.

9 For more details on the design principles, see Lars Buitinck et al., “API Design for Machine Learning Software: Experiences from the Scikit-Learn Project” ,” arXiv preprint arXiv:1309.0238 (2013).

10 Some predictors also provide methods to measure the confidence of their predictions.

11 By the time you read these lines, it may be possible to make all transformers output Pandas DataFrames when they receive a DataFrame as input: Pandas in, Pandas out. There will be a global configuration option for this: `sklearn.set_config(pandas_in_out=True).`

12 See SciPy’s documentation for more details.

13 In a nutshell, a REST (or RESTful) API is an HTTP-based API that follows some conventions, such as using standard HTTP verbs to read, update, create, or delete resources (GET, POST, PUT, and DELETE) and using JSON for the inputs and outputs.

14 A captcha is a test to ensure a user is not a robot. These tests have often been used as a cheap way to label training data.

Chapter 3. Classification

> **A NOTE FOR EARLY RELEASE READERS**
>
> With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.
>
> This will be the 3rd chapter of the final book. Notebooks are available on GitHub at *https://github.com/ageron/handson-ml3*. Datasets are available at *https://github.com/ageron/data*.
>
> If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the editoor at ntache@oreilly.com.

In Chapter 1 I mentioned that the most common supervised learning tasks are regression (predicting values) and classification (predicting classes). In Chapter 2 we explored a regression task, predicting housing values, using various algorithms such as Linear Regression, Decision Trees, and Random Forests (which will be explained in further detail in later chapters). Now we will turn our attention to classification systems.

MNIST

In this chapter we will be using the MNIST dataset, which is a set of 70,000 small images of digits handwritten by high school students and employees of the US Census Bureau. Each image is labeled with the digit it represents. This set has been studied so much that it is often called the "hello world" of Machine Learning: whenever people come up with a new classification algorithm they are curious to see how it will perform on MNIST, and anyone who learns Machine Learning tackles this dataset sooner or later.

Scikit-Learn provides many helper functions to download popular datasets. MNIST is one of them. The following code fetches the MNIST dataset from OpenML.org:[1]

```
from sklearn.datasets import fetch_openml

mnist = fetch_openml('mnist_784', as_frame=False)
```

The `sklearn.datasets` package contains mostly three types of functions: `fetch_*` functions such as `fetch_openml()` to download real-life datasets, `load_*` functions to load small toy datasets bundled with Scikit-Learn (so they don't need to be downloaded over the Internet), and `make_*` functions to generate fake datasets, useful for tests. Generated datasets are usually returned as an (X, y) tuple containing the input data and the targets, both as NumPy arrays. Other Datasets are returned as `sklearn.utils.Bunch` objects, which are dictionaries whose entries can also be accessed as attributes. They generally contain the following entries:

- `"DESCR"`: a description of the dataset
- `"data"`: the input data, usually as a 2D NumPy array
- `"target"`: the labels, usually as a 1D NumPy array

The `fetch_openml()` function is a bit unusual since by default it returns the inputs as a Pandas DataFrame and the labels as a Pandas Series (unless the dataset is sparse). But the MNIST dataset contains images, and DataFrames aren't ideal for that, so it's preferable to set `as_frame=False` to get the data as NumPy arrays instead. Let's look at these arrays:

```
>>> X, y = mnist.data, mnist.target
>>> X
array([[0., 0., 0., ..., 0., 0., 0.],
```

```
       [0., 0., 0., ..., 0., 0., 0.],
       [0., 0., 0., ..., 0., 0., 0.],
       ...,
       [0., 0., 0., ..., 0., 0., 0.],
       [0., 0., 0., ..., 0., 0., 0.],
       [0., 0., 0., ..., 0., 0., 0.]])
>>> X.shape
(70000, 784)
>>> y
array(['5', '0', '4', ..., '4', '5', '6'], dtype=object)
>>> y.shape
(70000,)
```

There are 70,000 images, and each image has 784 features. This is because each image is 28 × 28 pixels, and each feature simply represents one pixel's intensity, from 0 (white) to 255 (black). Let's take a peek at one digit from the dataset. All you need to do is grab an instance's feature vector, reshape it to a 28 × 28 array, and display it using Matplotlib's `imshow()` function (Figure 3-1). We use `cmap="binary"` to get a grayscale color map where 0 is white and 255 is black:

```
import matplotlib.pyplot as plt

def plot_digit(image_data):
    image = image_data.reshape(28, 28)
    plt.imshow(image, cmap="binary")
    plt.axis("off")

some_digit = X[0]
plot_digit(some_digit)
plt.show()
```

```
>>> X[0]
```

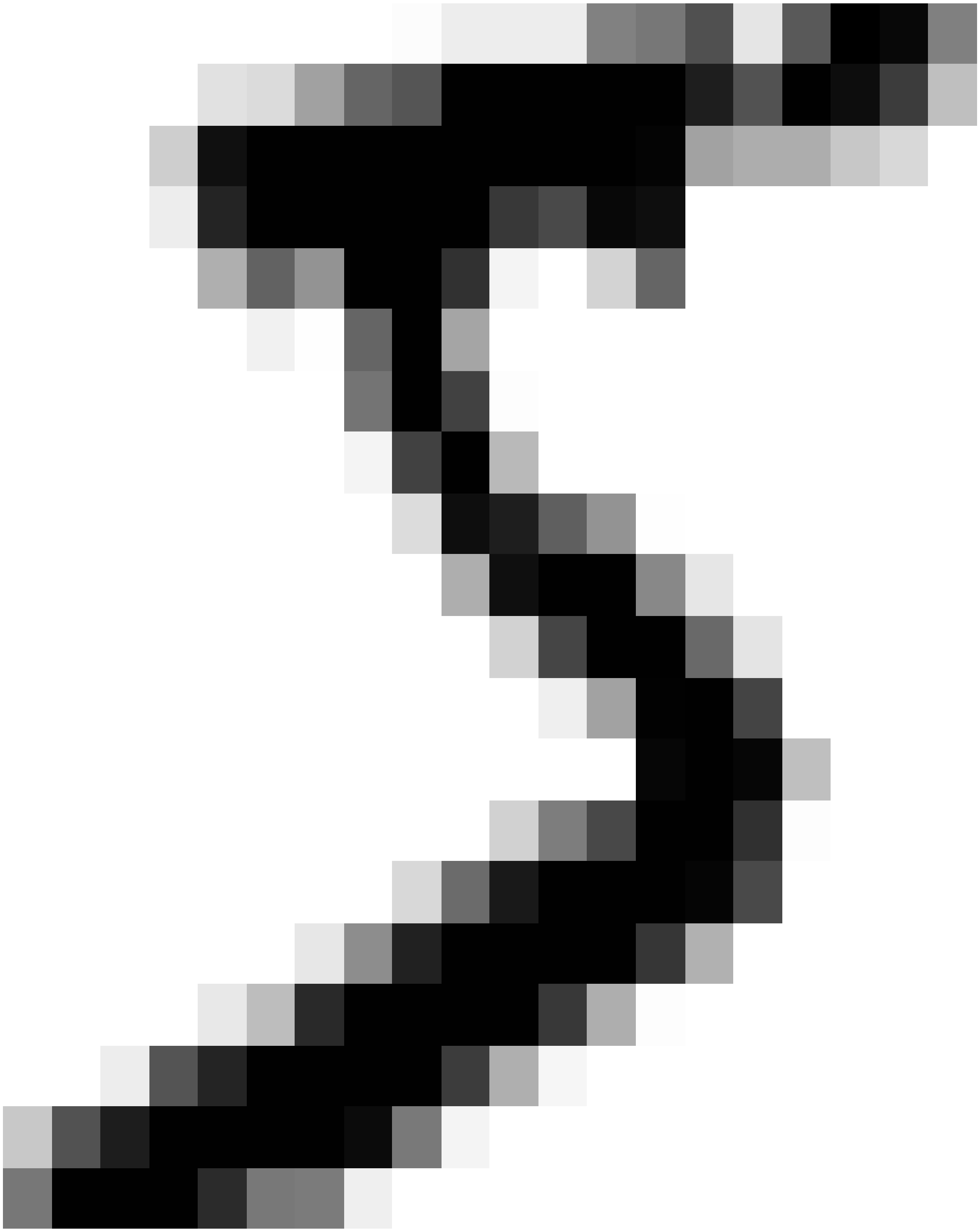


Figure 3-1. Example of an MNIST image

This looks like a 5, and indeed that's what the label tells us:

```
>>> y[0]
'5'
```

To give you a feel for the complexity of the classification task, Figure 3-2 shows a few more images from the MNIST dataset.

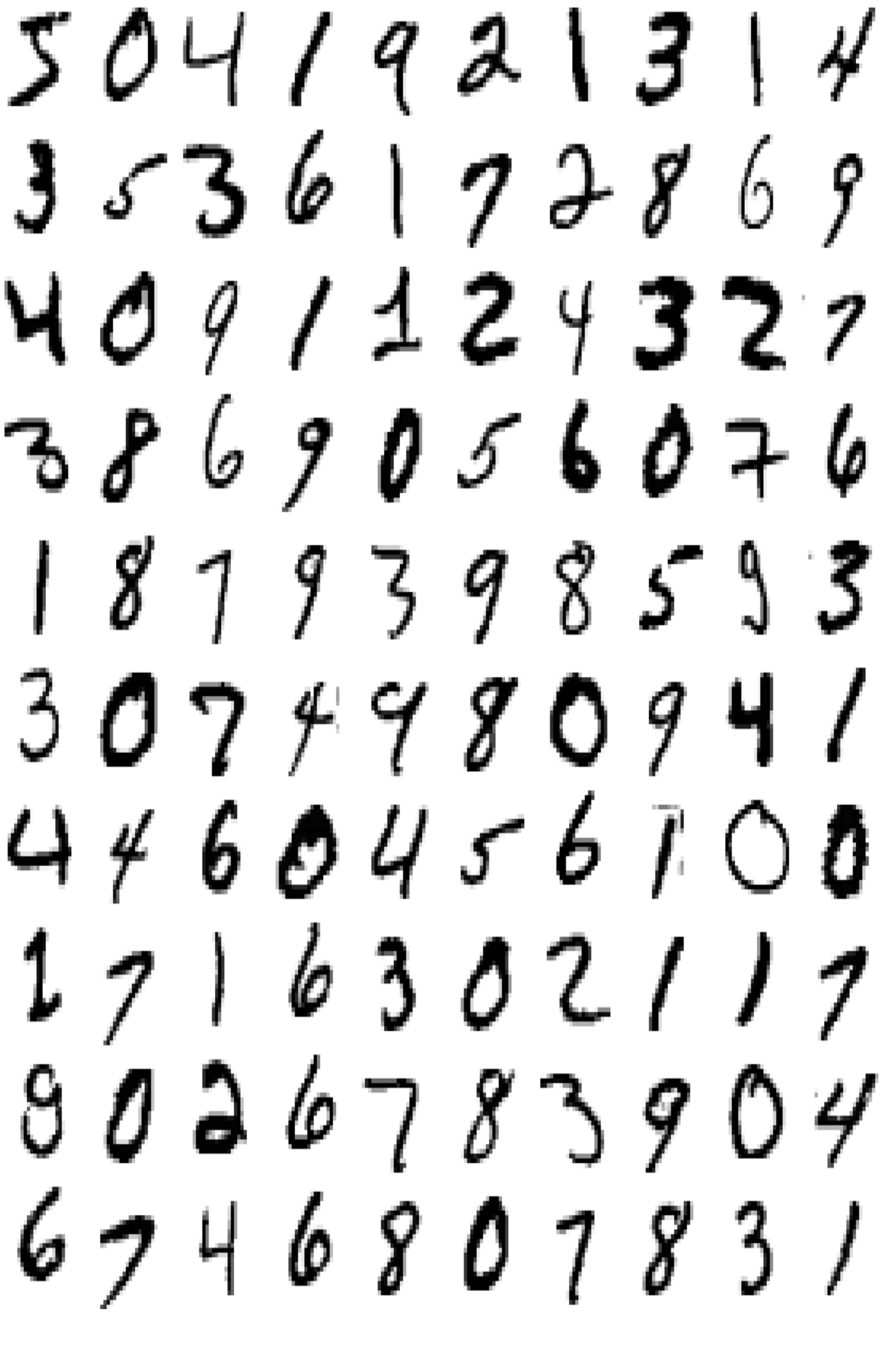


Figure 3-2. Digits from the MNIST dataset

But wait! You should always create a test set and set it aside before inspecting the data closely. The MNIST dataset returned by `fetch_openml()` is actually already split into a training set (the first 60,000 images) and a test set (the last 10,000 images):[2]

```
X_train, X_test, y_train, y_test = X[:60000], X[60000:],
y[:60000], y[60000:]
```

The training set is already shuffled for us, which is good because this guarantees that all cross-validation folds will be similar (you don't want one fold to be missing some digits). Moreover, some learning algorithms are sensitive to the order of the training instances, and they perform poorly if they get many similar instances in a row. Shuffling the dataset ensures that this won't happen.[3]

Training a Binary Classifier

Let's simplify the problem for now and only try to identify one digit—for example, the number 5. This "5-detector" will be an example of a *binary classifier*, capable of distinguishing between just two classes, 5 and not-5. Let's create the target vectors for this classification task:

```
y_train_5 = (y_train == '5')  # True for all 5s, False for all
other digits
y_test_5 = (y_test == '5')
```

Now let's pick a classifier and train it. A good place to start is with a *Stochastic Gradient Descent* (SGD) classifier, using Scikit-Learn's `SGDClassifier` class. This classifier is capable of handling very large datasets efficiently. This is in part because SGD deals with training instances independently, one at a time, which also makes SGD well suited for online learning, as we will see later. Let's create an `SGDClassifier` and train it on the whole training set:

```
from sklearn.linear_model import SGDClassifier

sgd_clf = SGDClassifier(random_state=42)
sgd_clf.fit(X_train, y_train_5)
```

Now we can use it to detect images of the number 5:

```
>>> sgd_clf.predict([some_digit])
array([ True])
```

The classifier guesses that this image represents a 5 (`True`). Looks like it guessed right in this particular case! Now, let's evaluate this model's performance.

Performance Measures

Evaluating a classifier is often significantly trickier than evaluating a regressor, so we will spend a large part of this chapter on this topic. There are many performance measures available, so grab another coffee and get ready to learn many new concepts and acronyms!

Measuring Accuracy Using Cross-Validation

A good way to evaluate a model is to use cross-validation, just as you did in Chapter 2. Let's use the `cross_val_score()` function to evaluate our `SGDClassifier` model, using K-fold cross-validation with three folds. Remember that K-fold cross-validation means splitting the training set into K folds (in this case, three), then training the model K times, holding out a different fold each time for evaluation (see Chapter 2):

```
>>> from sklearn.model_selection import cross_val_score
>>> cross_val_score(sgd_clf, X_train, y_train_5, cv=3,
scoring="accuracy")
array([0.95035, 0.96035, 0.9604 ])
```

Wow! Above 95% accuracy (ratio of correct predictions) on all cross-validation folds? This looks amazing, doesn't it? Well, before you get too excited, let's look at a dummy classifier that just classifies every single image in the most frequent class, in this case the negative class (i.e., *not* a 5):

```
from sklearn.dummy import DummyClassifier

dummy_clf = DummyClassifier()
dummy_clf.fit(X_train, y_train_5)
print(any(dummy_clf.predict(X_train)))  # prints False: no 5s
detected
```

Can you guess this model's accuracy? Let's find out:

```
>>> cross_val_score(dummy_clf, X_train, y_train_5, cv=3,
scoring="accuracy")
array([0.90965, 0.90965, 0.90965])
```

That's right, it has over 90% accuracy! This is simply because only about 10% of the images are 5s, so if you always guess that an image is *not* a 5, you will be right about 90% of the time. Beats Nostradamus.

This demonstrates why accuracy is generally not the preferred performance measure for classifiers, especially when you are dealing with *skewed datasets* (i.e., when some classes are much more frequent than others). A much better way to evaluate the performance of a classifier is to look at the *confusion matrix*.

IMPLEMENTING CROSS-VALIDATION

Occasionally you will need more control over the cross-validation process than what Scikit-Learn provides off the shelf. In these cases, you can implement cross-validation yourself. The following code does roughly the same thing as Scikit-Learn's `cross_val_score()` function, and it prints the same result:

```
from sklearn.model_selection import StratifiedKFold
from sklearn.base import clone

skfolds = StratifiedKFold(n_splits=3)  # add shuffle=True if
the dataset is not
                                       # already shuffled
for train_index, test_index in skfolds.split(X_train,
y_train_5):
    clone_clf = clone(sgd_clf)
    X_train_folds = X_train[train_index]
    y_train_folds = y_train_5[train_index]
    X_test_fold = X_train[test_index]
    y_test_fold = y_train_5[test_index]

    clone_clf.fit(X_train_folds, y_train_folds)
    y_pred = clone_clf.predict(X_test_fold)
    n_correct = sum(y_pred == y_test_fold)
    print(n_correct / len(y_pred))  # prints 0.95035, 0.96035
and 0.9604
```

The `StratifiedKFold` class performs stratified sampling (as explained in Chapter 2) to produce folds that contain a representative ratio of each class. At each iteration the code creates a clone of the classifier, trains that clone on the training folds, and makes predictions on the test fold. Then it counts the number of correct predictions and outputs the ratio of correct predictions.

Confusion Matrix

The general idea of a confusion matrix is to count the number of times instances of class A are classified as class B, for all A/B pairs. For example, to know the number of times the classifier confused images of 8s with 0s, you would look at row #8, column #0 of the confusion matrix.

To compute the confusion matrix, you first need to have a set of predictions so that they can be compared to the actual targets. You could make predictions on the test set, but let's keep it untouched for now (remember that you want to use the test set only at the very end of your project, once you have a classifier that you are ready to launch). Instead, you can use the `cross_val_predict()` function:

```
from sklearn.model_selection import cross_val_predict

y_train_pred = cross_val_predict(sgd_clf, X_train, y_train_5,
cv=3)
```

Just like the `cross_val_score()` function, `cross_val_predict()` performs K-fold cross-validation, but instead of returning the evaluation scores, it returns the predictions made on each test fold. This means that you get a clean prediction for each instance in the training set (by "clean" I mean "out-of-sample": the model makes predictions on data that it never saw during training).

Now you are ready to get the confusion matrix using the `confusion_matrix()` function. Just pass it the target classes (`y_train_5`) and the predicted classes (`y_train_pred`):

```
>>> from sklearn.metrics import confusion_matrix
>>> cm = confusion_matrix(y_train_5, y_train_pred)
>>> cm
array([[53892,   687],
       [ 1891,  3530]])
```

Each row in a confusion matrix represents an *actual class*, while each column represents a *predicted class*. The first row of this matrix considers non-5 images (the *negative class*): 53,892 of them were correctly classified as non-5s (they are called *true negatives*), while the remaining 687 were wrongly classified as 5s (*false positives*, also called *type I errors*). The second row considers the images of 5s (the *positive class*): 1,891 were wrongly classified as non-5s (*false negatives*, also called *type II errors*), while the remaining 3,530 were correctly classified as 5s (*true positives*). A perfect classifier would only have true positives and true negatives, so its confusion matrix would have nonzero values only on its main diagonal (top left to bottom right):

```
>>> y_train_perfect_predictions = y_train_5  # pretend we reached perfection
>>> confusion_matrix(y_train_5, y_train_perfect_predictions)
array([[54579,     0],
       [    0,  5421]])
```

The confusion matrix gives you a lot of information, but sometimes you may prefer a more concise metric. An interesting one to look at is the accuracy of the positive predictions; this is called the *precision* of the classifier (Equation 3-1).

Equation 3-1. Precision

$$\text{precision} = \frac{TP}{TP + FP}$$

TP is the number of true positives, and *FP* is the number of false positives.

A trivial way to have perfect precision is to create a classifier that always makes negative predictions, except for one single positive prediction on the instance it's most confident about. If this one prediction is correct, then the classifier has 100% precision (precision = 1/1 = 100%). Obviously, such a classifier would not be very useful, since it would ignore all but one positive instance. So precision is typically used along with another metric named *recall*, also called *sensitivity* or the *true positive rate* (TPR): this is the ratio of positive instances that are correctly detected by the classifier (Equation 3-2).

Equation 3-2. Recall

$$\text{recall} = \frac{TP}{TP + FN}$$

FN is, of course, the number of false negatives.

If you are confused about the confusion matrix, Figure 3-3 may help.

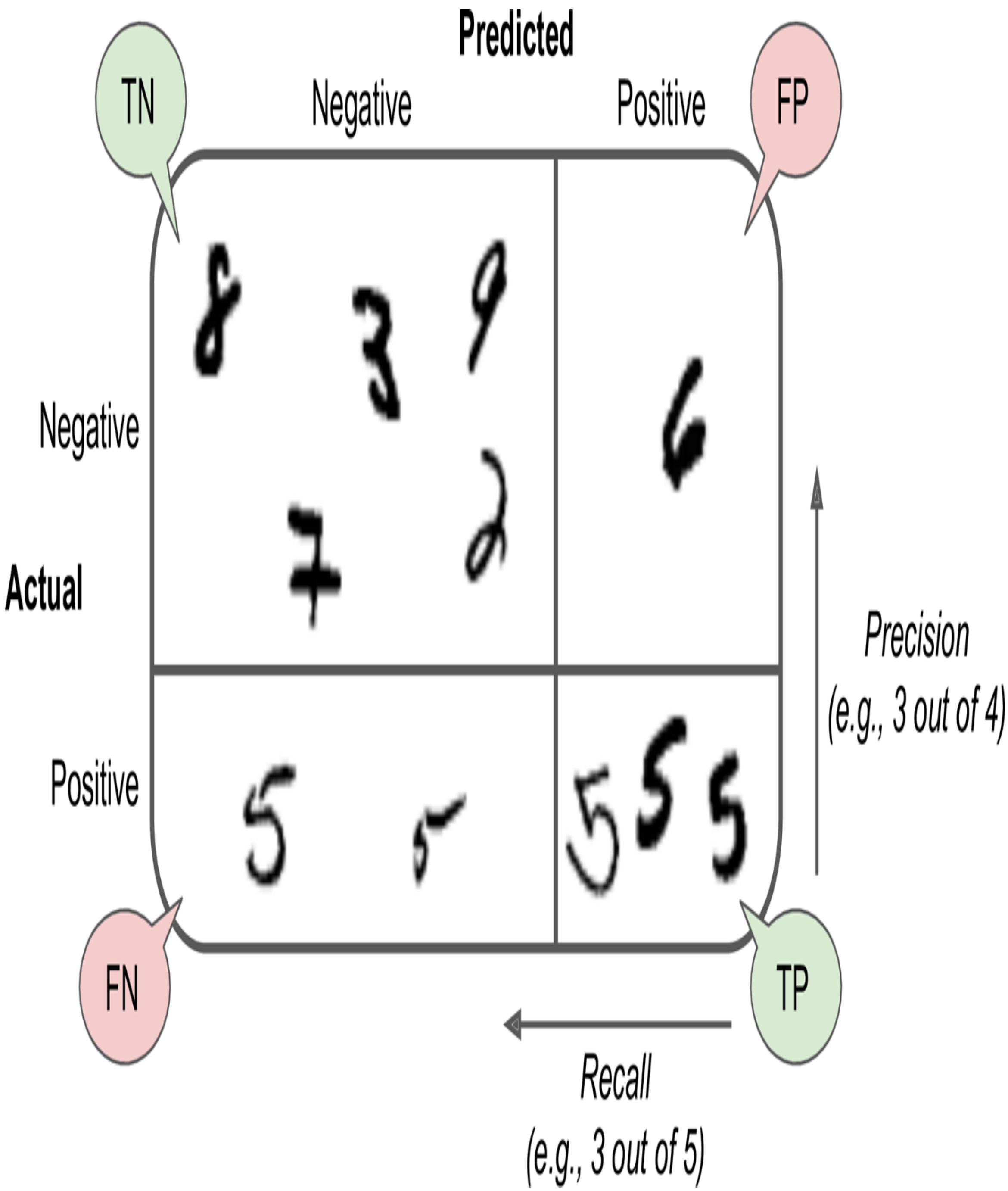


Figure 3-3. An illustrated confusion matrix shows examples of true negatives (top left), false positives (top right), false negatives (lower left), and true positives (lower right)

Precision and Recall

Scikit-Learn provides several functions to compute classifier metrics, including precision and recall:

```
>>> from sklearn.metrics import precision_score, recall_score
>>> precision_score(y_train_5, y_train_pred)  # == 3530 / (687 +
3530)
0.8370879772350012
>>> recall_score(y_train_5, y_train_pred)  # == 3530 / (1891 +
3530)
0.6511713705958311
```

Now your 5-detector does not look as shiny as it did when you looked at its accuracy. When it claims an image represents a 5, it is correct only 83.7% of the time. Moreover, it only detects 65.1% of the 5s.

It is often convenient to combine precision and recall into a single metric called the *F_1 score*, especially when you need a single metric to compare two classifiers. The F_1 score is the *harmonic mean* of precision and recall (Equation 3-3). Whereas the regular mean treats all values equally, the harmonic mean gives much more weight to low values. As a result, the classifier will only get a high F_1 score if both recall and precision are high.

Equation 3-3. F_1 score

$$F_1 = \frac{2}{\frac{1}{\text{precision}} + \frac{1}{\text{recall}}} = 2 \times \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}} = \frac{TP}{TP + \frac{FN+FP}{2}}$$

To compute the F_1 score, simply call the `f1_score()` function:

```
>>> from sklearn.metrics import f1_score
>>> f1_score(y_train_5, y_train_pred)
0.7325171197343846
```

The F_1 score favors classifiers that have similar precision and recall. This is not always what you want: in some contexts you mostly care about precision, and in other contexts you really care about recall. For example, if you trained a classifier to detect videos that are safe for kids, you would probably prefer a classifier that rejects many good videos (low recall) but keeps only safe ones (high precision), rather than a classifier that has a much higher recall but lets a few really bad videos show up in your product (in such cases, you may even want to add a human pipeline to check the classifier's video selection). On the other hand, suppose you train a classifier to detect shoplifters in surveillance images: it is probably fine if your classifier only has 30% precision as long as it has 99% recall (sure, the security guards will get a few false alerts, but almost all shoplifters will get caught).

Unfortunately, you can't have it both ways: increasing precision reduces recall, and vice versa. This is called the *precision/recall trade-off*.

Precision/Recall Trade-off

To understand this trade-off, let's look at how the `SGDClassifier` makes its classification decisions. For each instance, it computes a score based on a *decision function*. If that score is greater than a threshold, it assigns the instance to the positive class; otherwise it assigns it to the negative class. Figure 3-4 shows a few digits positioned from the lowest score on the left to the highest score on the right. Suppose the *decision threshold* is positioned at the central arrow (between the two 5s): you will find 4 true positives (actual 5s) on the right of that threshold, and 1 false positive (actually a 6). Therefore, with that threshold, the precision is 80% (4 out of 5). But out of 6 actual 5s, the classifier only detects 4, so the recall is 67% (4 out of 6). If you raise the threshold (move it to the arrow on the right), the false positive (the 6) becomes a true negative, thereby increasing the precision (up to 100% in this case), but one true positive becomes a false negative, decreasing recall down to 50%. Conversely, lowering the threshold increases recall and reduces precision.

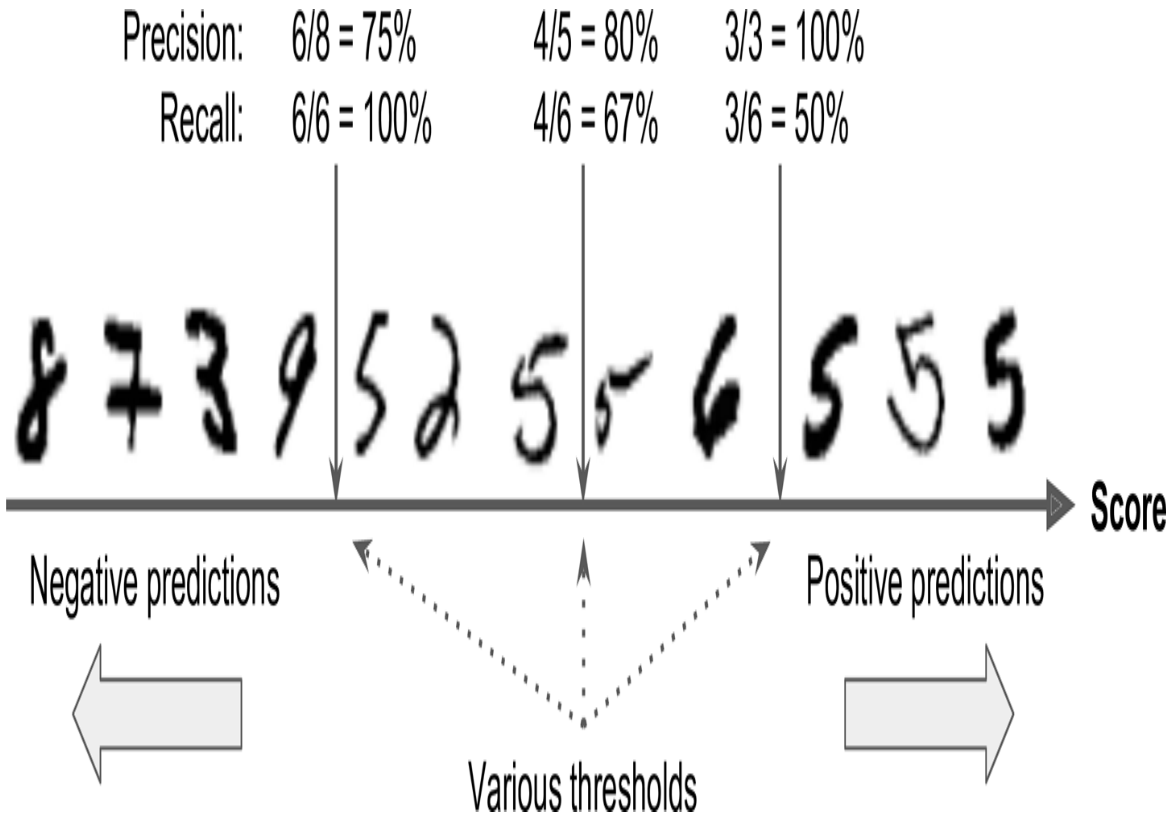


Figure 3-4. In this precision/recall trade-off, images are ranked by their classifier score, and those above the chosen decision threshold are considered positive; the higher the threshold, the lower the recall, but (in general) the higher the precision

Scikit-Learn does not let you set the threshold directly, but it does give you access to the decision scores that it uses to make predictions. Instead of calling the classifier's `predict()` method, you can call its `decision_function()` method, which returns a score for each instance, and then use any threshold you want to make predictions based on those scores:

```
>>> y_scores = sgd_clf.decision_function([some_digit])
>>> y_scores
array([2164.22030239])
>>> threshold = 0
>>> y_some_digit_pred = (y_scores > threshold)
array([ True])
```

The `SGDClassifier` uses a threshold equal to 0, so the previous code returns the same result as the `predict()` method (i.e., `True`). Let's raise the threshold:

```
>>> threshold = 3000
>>> y_some_digit_pred = (y_scores > threshold)
>>> y_some_digit_pred
array([False])
```

This confirms that raising the threshold decreases recall. The image actually represents a 5, and the classifier detects it when the threshold is 0, but it misses it when the threshold is increased to 3,000.

How do you decide which threshold to use? First, use the `cross_val_predict()` function to get the scores of all instances in the training set, but this time specify that you want to return decision scores instead of predictions:

```
y_scores = cross_val_predict(sgd_clf, X_train, y_train_5, cv=3,
                             method="decision_function")
```

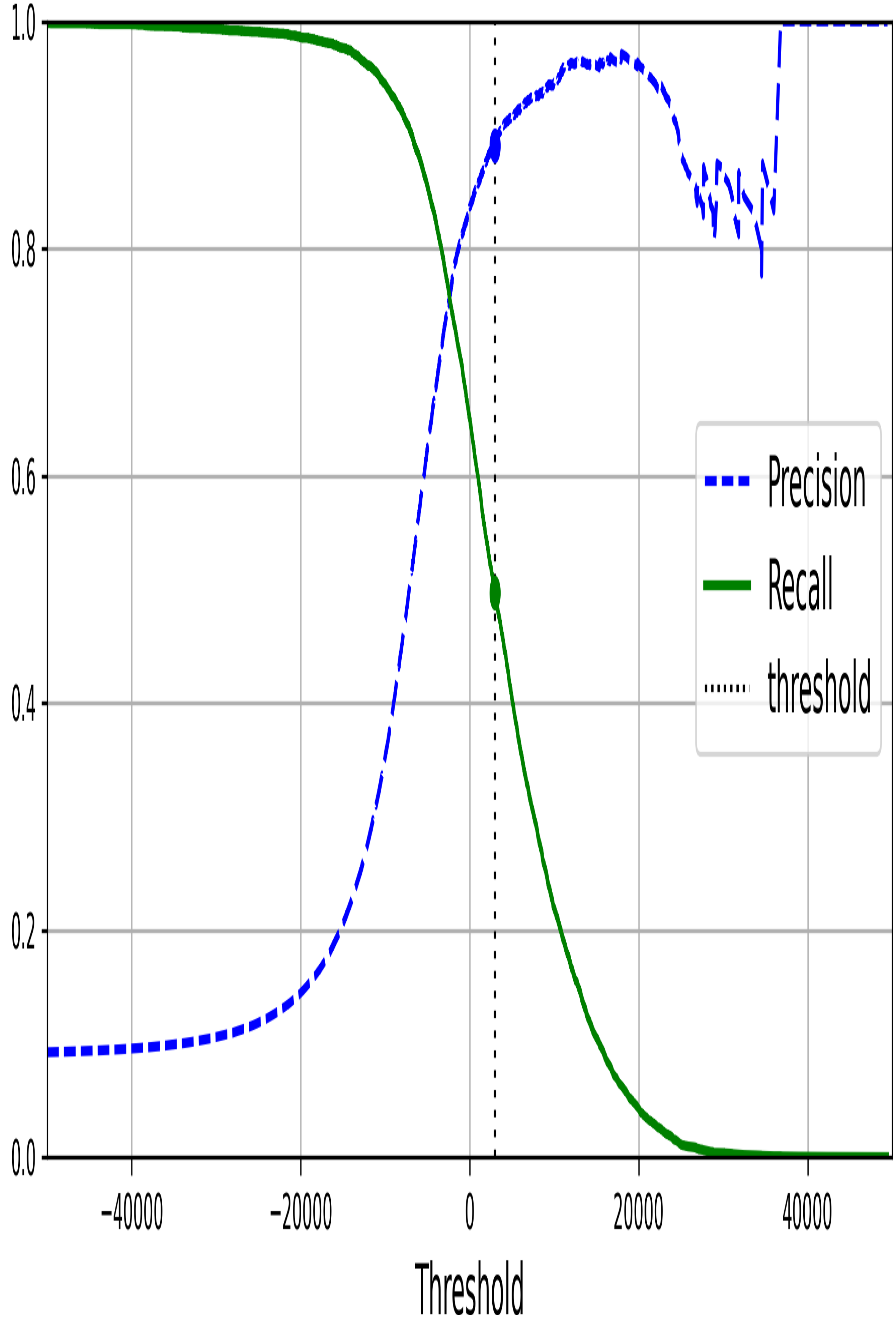
With these scores, use the `precision_recall_curve()` function to compute precision and recall for all possible thresholds (the function adds a last precision of 0 and a last recall of 1, corresponding to an infinite threshold):

```
from sklearn.metrics import precision_recall_curve

precisions, recalls, thresholds =
precision_recall_curve(y_train_5, y_scores)
```

Finally, use Matplotlib to plot precision and recall as functions of the threshold value (Figure 3-5), and let's show the threshold of 3,000 we selected:

```
plt.plot(thresholds, precisions[:-1], "b--", label="Precision",
linewidth=2)
plt.plot(thresholds, recalls[:-1], "g-", label="Recall",
linewidth=2)
plt.vlines(threshold, 0, 1.0, "k", "dotted", label="threshold")
[...]  # beautify the figure: add grid, legend, axis, labels and
```

```
circles
plt.show()
```



1.0
0.8
0.6
0.4
0.2
0.0
−40000
−20000
0
20000
40000
Threshold
Precision
Recall
threshold

Figure 3-5. Precision and recall versus the decision threshold

> **NOTE**
>
> You may wonder why the precision curve is bumpier than the recall curve in Figure 3-5. The reason is that precision may sometimes go down when you raise the threshold (although in general it will go up). To understand why, look back at Figure 3-4 and notice what happens when you start from the central threshold and move it just one digit to the right: precision goes from 4/5 (80%) down to 3/4 (75%). On the other hand, recall can only go down when the threshold is increased, which explains why its curve looks smooth.

At this threshold value, precision is near 90% and recall is around 50%. Another way to select a good precision/recall trade-off is to plot precision directly against recall, as shown in Figure 3-6 (the same threshold is shown).

```
plt.plot(recalls, precisions, linewidth=2,
label="Precision/Recall curve")
[...]  # beautify the figure: add labels, grid, legend, arrow and
text
plt.show()
```

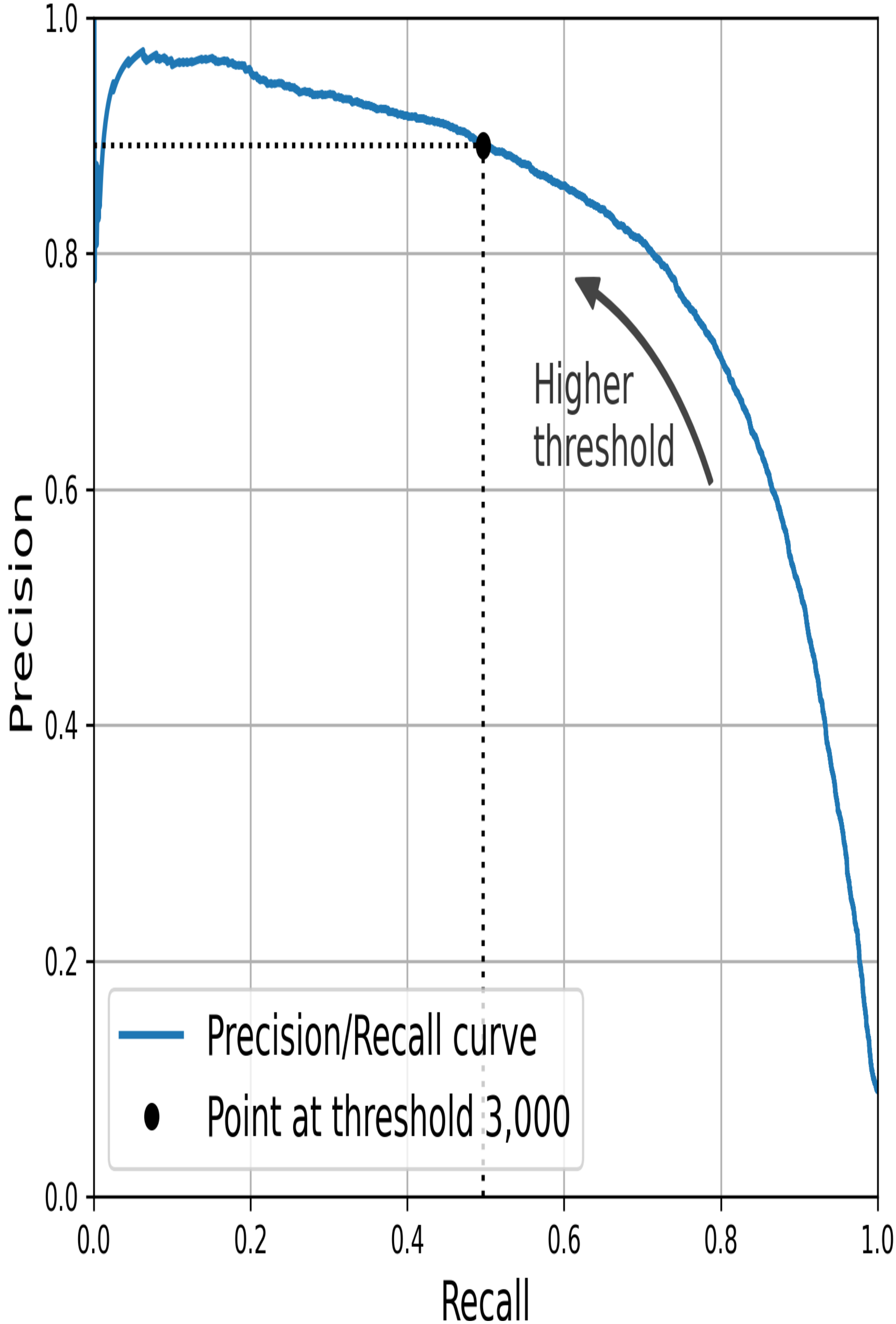

Precision
Recall
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
Higher
threshold
Precision/Recall curve
Point at threshold 3,000

Figure 3-6. Precision versus recall

You can see that precision really starts to fall sharply around 80% recall. You will probably want to select a precision/recall trade-off just before that drop—for example, at around 60% recall. But of course, the choice depends on your project.

Suppose you decide to aim for 90% precision. You could use the first plot to find the threshold you need to use, but that's not very precise. Alternatively, you can search for the lowest threshold that gives you at least 90% precision. For this, we can use NumPy array's `argmax()` method, which returns the first index of the maximum value, which in this case means the first `True` value:

```
>>> idx_for_90_precision = (precisions >= 0.90).argmax()
>>> threshold_for_90_precision = thresholds[idx_for_90_precision]
>>> threshold_for_90_precision
3370.0194991439557
```

To make predictions (on the training set for now), instead of calling the classifier's `predict()` method, you can run this code:

```
y_train_pred_90 = (y_scores >= threshold_for_90_precision)
```

Let's check these predictions' precision and recall:

```
>>> precision_score(y_train_5, y_train_pred_90)
0.9000345901072293
>>> recall_at_90_precision = recall_score(y_train_5,
y_train_pred_90)
>>> recall_at_90_precision
0.4799852425751706
```

Great, you have a 90% precision classifier! As you can see, it is fairly easy to create a classifier with virtually any precision you want: just set a high enough threshold, and you're done. But wait, not so fast: a high-precision classifier is not very useful if its recall is too low! For many applications, 48% recall wouldn't be great at all.

TIP

If someone says, "Let's reach 99% precision," you should ask, "At what recall?"

The ROC Curve

The *receiver operating characteristic* (ROC) curve is another common tool used with binary classifiers. It is very similar to the precision/recall curve, but instead of plotting precision versus recall, the ROC curve plots the *true positive rate* (another name for recall) against the *false positive rate* (FPR). The FPR (also called the *fall-out*) is the ratio of negative instances that are incorrectly classified as positive. It is equal to 1 – the *true negative rate* (TNR), which is the ratio of negative instances that are correctly classified as negative. The TNR is also called *specificity*. Hence, the ROC curve plots *sensitivity* (recall) versus 1 – *specificity*.

To plot the ROC curve, you first use the `roc_curve()` function to compute the TPR and FPR for various threshold values:

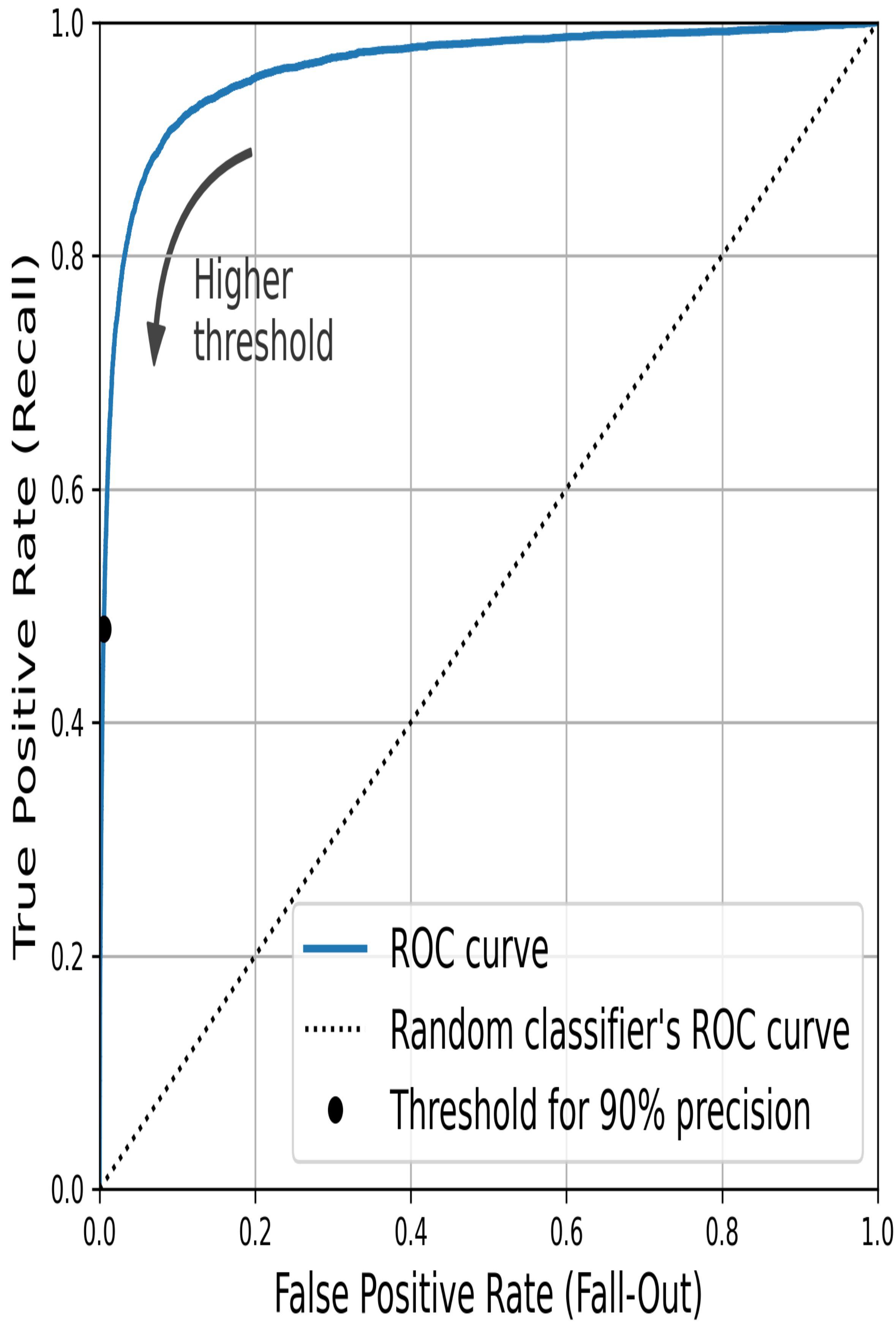
```
from sklearn.metrics import roc_curve

fpr, tpr, thresholds = roc_curve(y_train_5, y_scores)
```

Then you can plot the FPR against the TPR using Matplotlib. The following code produces the plot in Figure 3-7. To find the point that corresponds to 90% precision, we need to look for the index of the desired threshold. Since thresholds are listed in decreasing order in this case, we use <= instead of >= on the first line:

```
idx_for_threshold_at_90 = (thresholds <=
threshold_for_90_precision).argmax()
tpr_90, fpr_90 = tpr[idx_for_threshold_at_90],
fpr[idx_for_threshold_at_90]

plt.plot(fpr, tpr, linewidth=2, label="ROC curve")
plt.plot([0, 1], [0, 1], 'k:', label="Random classifier's ROC
curve")
plt.plot([fpr_90], [tpr_90], "ko", label="Threshold for 90%
```

```
precision")
[...]  # beautify the figure: add labels, grid, legend, arrow and
text
plt.show()
```

Once again there is a trade-off: the higher the recall (TPR), the more false positives (FPR) the classifier produces. The dotted line represents the ROC curve of a purely random classifier; a good classifier stays as far away from that line as possible (toward the top-left corner).



True Positive Rate (Recall)
False Positive Rate (Fall-Out)
Higher threshold
ROC curve
Random classifier's ROC curve
Threshold for 90% precision
0.0
0.2
0.4
0.6
0.8
1.0

Figure 3-7. This ROC curve plots the false positive rate against the true positive rate for all possible thresholds; the black circle highlights the chosen ratio (at 90% precision and 48% recall)

One way to compare classifiers is to measure the *area under the curve* (AUC). A perfect classifier will have a ROC AUC equal to 1, whereas a purely random classifier will have a ROC AUC equal to 0.5. Scikit-Learn provides a function to estimate the ROC AUC:

```
>>> from sklearn.metrics import roc_auc_score
>>> roc_auc_score(y_train_5, y_scores)
0.9604938554008616
```

> **TIP**
>
> Since the ROC curve is so similar to the precision/recall (PR) curve, you may wonder how to decide which one to use. As a rule of thumb, you should prefer the PR curve whenever the positive class is rare or when you care more about the false positives than the false negatives. Otherwise, use the ROC curve. For example, looking at the previous ROC curve (and the ROC AUC score), you may think that the classifier is really good. But this is mostly because there are few positives (5s) compared to the negatives (non-5s). In contrast, the PR curve makes it clear that the classifier has room for improvement: the curve could really be closer to the top-right corner (see Figure 3-6 again).

Let's now create a `RandomForestClassifier`, and we will compare its PR curve and F_1 score to those of the `SGDClassifier`:

```
from sklearn.ensemble import RandomForestClassifier

forest_clf = RandomForestClassifier(random_state=42)
```

The `precision_recall_curve()` function expects labels and scores for each instance, so we need to train the random forest and make it assign a score to each instance. But the `RandomForestClassifier` class does not have a `decision_function()` method, due to the way it works (we will cover this in Chapter 7). Luckily, it has a `predict_proba()` method which returns class probabilities for each instance, and we can just use the probability of the positive class as a score, it will work fine.[4] So let's call the `cross_val_predict()` function to train the `RandomForestClassifier` using cross-validation and make it predict class probabilities for every image:

```
y_probas_forest = cross_val_predict(forest_clf, X_train,
y_train_5, cv=3,
                                    method="predict_proba")
```

Let's look at the class probabilities for the first two images in the training set:

```
>>> y_probas_forest[:2]
array([[0.11, 0.89],
       [0.99, 0.01]])
```

The model predicts that the first image is positive with 89% probability, and it predicts that the second image is negative with 99% probability. Since each image is either positive or negative, the probabilities in each row add up to 100%.

WARNING

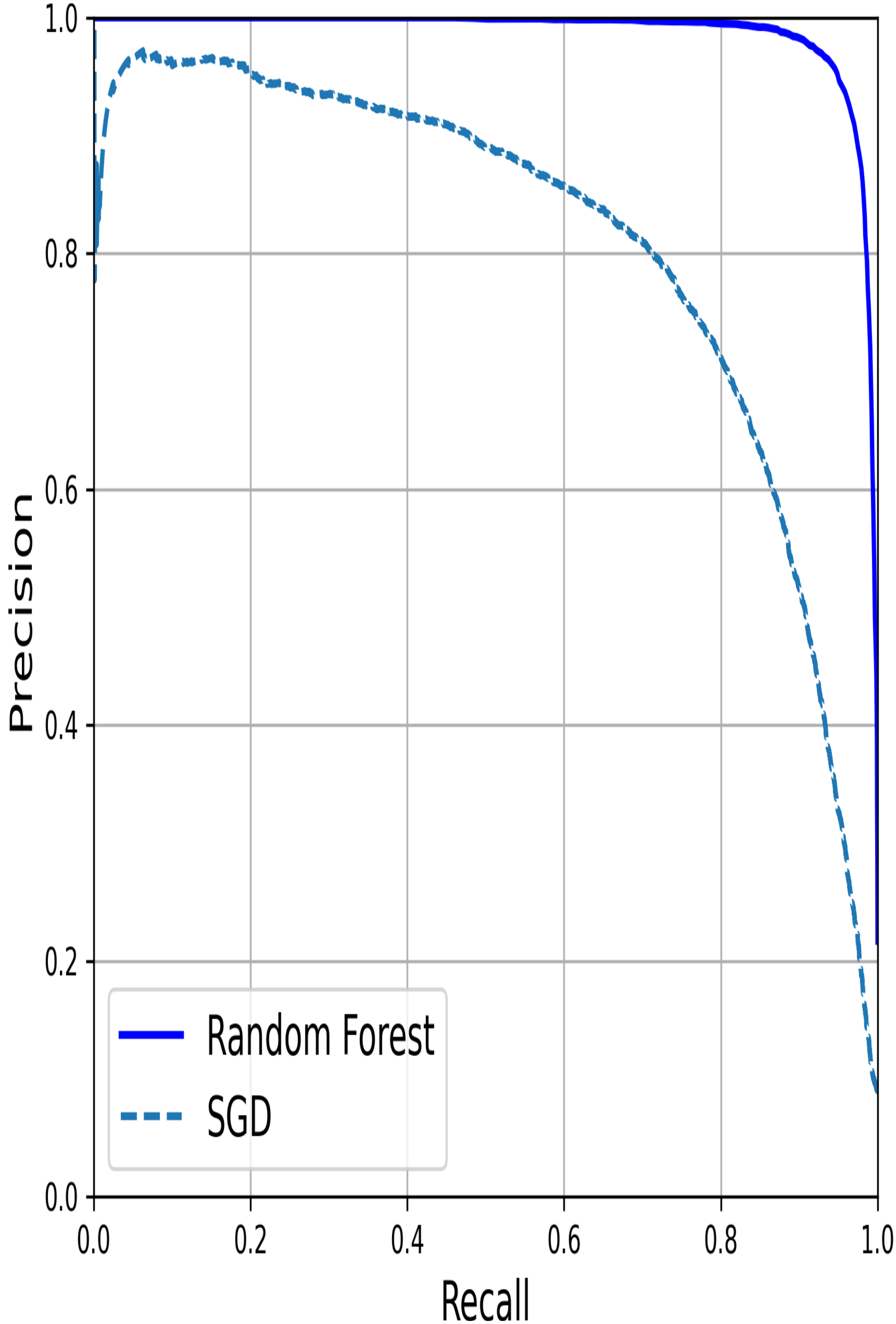
These are *estimated* probabilities, not actual probabilities. For example, if you look at all the images that the model classified as positive with an estimated probability between 50% and 60%, roughly 94% of them are actually positive. So the model's estimated probabilities were much too low in this case—but models can be overconfident as well. The `sklearn.calibration` package contains tools to calibrate the estimated probabilities and make them much closer to actual probabilities. See the extra material section in the notebook for more details.

The second column contains the estimated probabilities for the positive class, so let's pass them to the `precision_recall_curve()` function:

```
y_scores_forest = y_probas_forest[:, 1]
precisions_forest, recalls_forest, thresholds_forest =
precision_recall_curve(
    y_train_5, y_scores_forest)
```

Now you are ready to plot the PR curve. It is useful to plot the first PR curve as well to see how they compare (Figure 3-8):

```
plt.plot(recalls_forest, precisions_forest, "b-", linewidth=2,
         label="Random Forest")
plt.plot(recalls, precisions, "--", linewidth=2, label="SGD")
[...]  # beautify the figure: add labels, grid, and legend
plt.show()
```



Precision
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
Recall
Random Forest
SGD

Figure 3-8. Comparing PR curves: the Random Forest classifier is superior to the SGD classifier because its PR curve is much closer to the top-right corner, and it has a greater AUC

As you can see in Figure 3-8, the `RandomForestClassifier`'s PR curve looks much better than the `SGDClassifier`'s: it comes much closer to the top-right corner. Its F_1 score and ROC AUC score are also significantly better:

```
>>> y_train_pred_forest = y_probas_forest[:, 1] >= 0.5  #
positive proba ≥ 50%
>>> f1_score(y_train_5, y_pred_forest)
0.9242275142688446
>>> roc_auc_score(y_train_5, y_scores_forest)
0.9983436731328145
```

Try measuring the precision and recall scores: you should find about 99.1% precision and 86.6% recall. Not too bad!

You now know how to train binary classifiers, choose the appropriate metric for your task, evaluate your classifiers using cross-validation, select the precision/recall trade-off that fits your needs, and use several metrics and curves to compare various models. Now let's try to detect more than just the 5s.

Multiclass Classification

Whereas binary classifiers distinguish between two classes, *multiclass classifiers* (also called *multinomial classifiers*) can distinguish between more than two classes.

Some Scikit-Learn classifiers, such as `LogisticRegression`, `RandomForestClassifier`, and `GaussianNB`, are capable of handling multiple classes natively. Others, such as `SGDClassifier` or `SVC`, are strictly binary classifiers. However, there are various strategies that you can use to perform multiclass classification with multiple binary classifiers.

One way to create a system that can classify the digit images into 10 classes (from 0 to 9) is to train 10 binary classifiers, one for each digit (a 0-detector, a 1-detector, a 2-detector, and so on). Then when you want to classify an image, you get the decision score from each classifier for that image and you select the class whose classifier outputs the highest score. This is called the *one-versus-the-rest* (OvR) strategy (also called *one-versus-all*).

Another strategy is to train a binary classifier for every pair of digits: one to distinguish 0s and 1s, another to distinguish 0s and 2s, another for 1s and 2s, and so on. This is called the *one-versus-one* (OvO) strategy. If there are N classes, you need to train $N \times (N - 1) / 2$ classifiers. For the MNIST problem, this means training 45 binary classifiers! When you want to classify an image, you have to run the image through all 45 classifiers and see which class wins the most duels. The main advantage of OvO is that each classifier only needs to be trained on the part of the training set for the two classes that it must distinguish.

Some algorithms (such as Support Vector Machine classifiers) scale poorly with the size of the training set. For these algorithms OvO is preferred because it is faster to train many classifiers on small training sets than to train few classifiers on large training sets. For most binary classification algorithms, however, OvR is preferred.

Scikit-Learn detects when you try to use a binary classification algorithm for a multiclass classification task, and it automatically runs OvR or OvO, depending on the algorithm. Let's try this with a Support Vector Machine classifier using the `sklearn.svm.SVC` class (see Chapter 5). We'll only train on the first 2,000 images or else it will take a very long time:

```
from sklearn.svm import SVC

svm_clf = SVC(random_state=42)
svm_clf.fit(X_train[:2000], y_train[:2000])  # y_train, not
y_train_5
```

That was easy! We trained the `SVC` using the original target classes from 0 to 9 (`y_train`), instead of the 5-versus-the-rest target classes (y_train_5). Since there are 10 classes, more than 2, Scikit-Learn used the OvO strategy: it trained 45 binary classifiers. Now let's make a prediction on an image:

```
>>> svm_clf.predict([some_digit])
array(['5'], dtype=object)
```

That's correct! This code actually made 45 predictions—one per pair of classes—and it selected the class that won the most duels. If you call the decision_function() method, you will see that it returns 10 scores per instance: one per class. Each class gets a score equal to the number of won duels plus or minus a small tweak (max ±0.33) to break ties, based on the classifier scores:

```
>>> some_digit_scores = svm_clf.decision_function([some_digit])
>>> some_digit_scores.round(2)
array([[ 3.79,  0.73,  6.06,  8.3 , -0.29,  9.3 ,  1.75,  2.77,
7.21,
         4.82]])
```

The highest score is 9.3, and it's indeed the one corresponding to class 5:

```
>>> class_id = some_digit_scores.argmax()
>>> class_id
5
```

When a classifier is trained, it stores the list of target classes in its classes_ attribute, ordered by value. In the case of MNIST, the index of each class in the classes_ array conveniently matches the class itself (e.g., the class at index 5 happens to be class '5'), but in general you won't be so lucky: you will need to look up the class label like this:

```
>>> svm_clf.classes_
array(['0', '1', '2', '3', '4', '5', '6', '7', '8', '9'],
dtype=object)
>>> svm_clf.classes_[class_id]
'5'
```

If you want to force Scikit-Learn to use one-versus-one or one-versus-the-rest, you can use the `OneVsOneClassifier` or `OneVsRestClassifier` classes. Simply create an instance and pass a classifier to its constructor (it does not even have to be a binary classifier). For example, this code creates a multiclass classifier using the OvR strategy, based on an `SVC`:

```
from sklearn.multiclass import OneVsRestClassifier

ovr_clf = OneVsRestClassifier(SVC(random_state=42))
ovr_clf.fit(X_train[:2000], y_train[:2000])
```

Let's make a prediction, and check the number of trained classifiers:

```
>>> ovr_clf.predict([some_digit])
array(['5'], dtype='<U1')
>>> len(ovr_clf.estimators_)
10
```

Training an `SGDClassifier` on a multiclass dataset and using it to make predictions is just as easy:

```
>>> sgd_clf = SGDClassifier(random_state=42)
>>> sgd_clf.fit(X_train, y_train)
>>> sgd_clf.predict([some_digit])
array(['3'], dtype='<U1')
```

Oops, that's incorrect. Prediction errors do happen! This time Scikit-Learn used the OvR strategy under the hood: since there are 10 classes, it trained 10 binary classifiers. The `decision_function()` method now returns one value per class. Let's look at the score that the SGD classifier assigned to each class:

```
>>> sgd_clf.decision_function([some_digit]).round()
array([[-31893., -34420.,  -9531.,   1824., -22320.,  -1386.,
-26189.,
        -16148.,  -4604., -12051.]])
```

You can see that the classifier is not very confident about its prediction: almost all scores are very negative, while class 3 has a score of +1,824, and class 5 is not too far behind at –1,386. Now of course you want to evaluate this classifier on more than one image. Since there are roughly as many images of each class, the accuracy metric is fine. As usual, you can use the `cross_val_score()` function to evaluate the model:

```
>>> cross_val_score(sgd_clf, X_train, y_train, cv=3,
scoring="accuracy")
array([0.87365, 0.85835, 0.8689 ])
```

It gets over 85.8% on all test folds. If you used a random classifier, you would get 10% accuracy, so this is not such a bad score, but you can still do much better. Simply scaling the inputs (as discussed in Chapter 2) increases accuracy above 89.1%:

```
>>> from sklearn.preprocessing import StandardScaler
>>> scaler = StandardScaler()
>>> X_train_scaled =
scaler.fit_transform(X_train.astype("float64"))
>>> cross_val_score(sgd_clf, X_train_scaled, y_train, cv=3,
scoring="accuracy")
array([0.8983, 0.891 , 0.9018])
```

Error Analysis

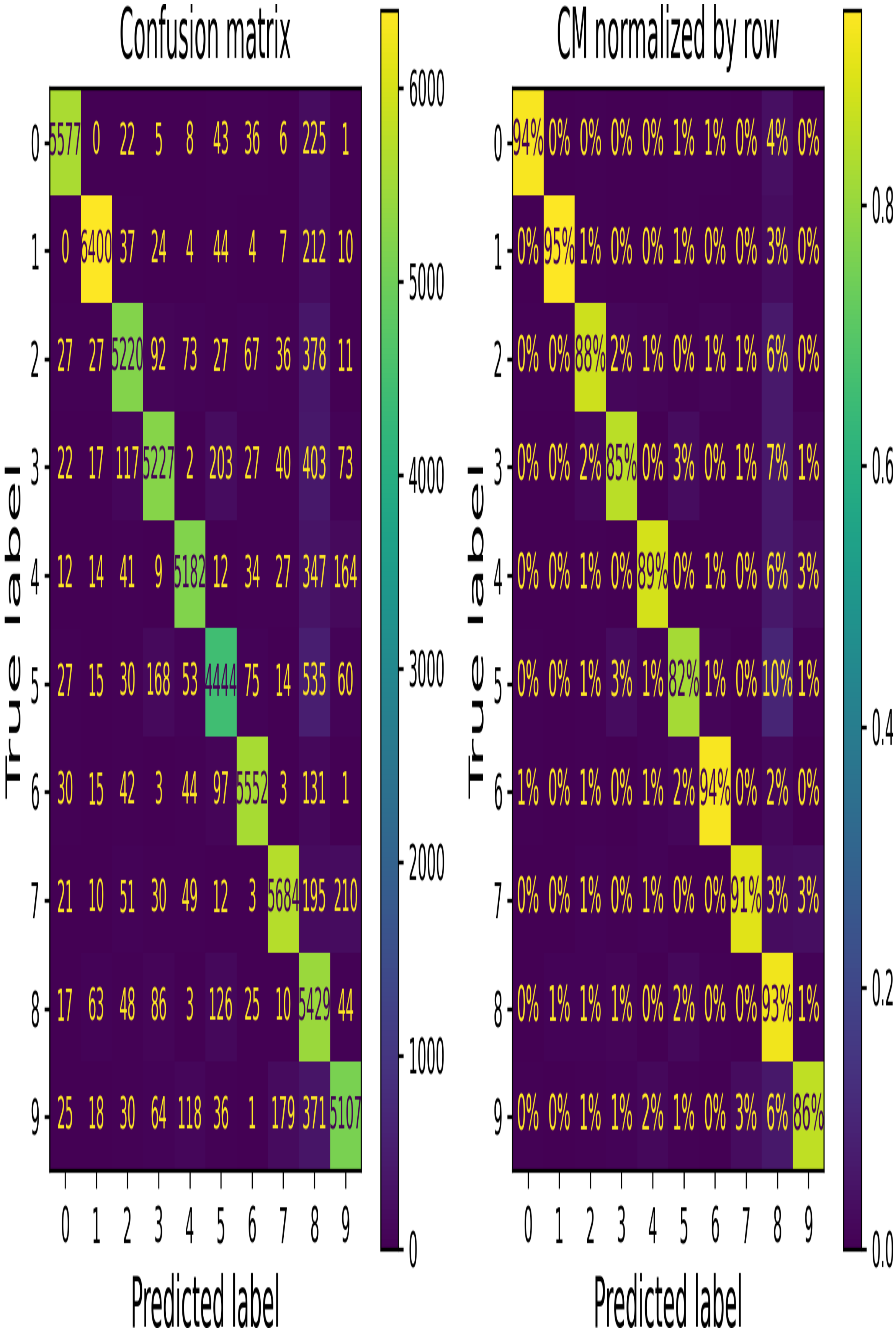
If this were a real project, you would now follow the steps in your Machine Learning project checklist (see Appendix A). You'd explore data preparation options, try out multiple models, shortlist the best ones, fine-tune their hyperparameters using `GridSearchCV`, and automate as much as possible. Here, we will assume that you have found a promising model and you want to find ways to improve it. One way to do this is to analyze the types of errors it makes.

First, look at the confusion matrix. For this, you first need to make predictions using the `cross_val_predict()` function, then you can pass the labels and predictions to the `confusion_matrix()` function, just like you did earlier. However, since there are now 10 classes instead of 2, the confusion matrix will contain quite a lot of numbers, and it may be hard to read. A colored diagram of the confusion matrix is much easier to analyze. To plot such a diagram, you can use the `ConfusionMatrixDisplay.from_predictions()` function like this:

```
from sklearn.metrics import ConfusionMatrixDisplay

y_train_pred = cross_val_predict(sgd_clf, X_train_scaled,
y_train, cv=3)
ConfusionMatrixDisplay.from_predictions(y_train, y_train_pred)
plt.show()
```

This produces the left diagram in Figure 3-9. This confusion matrix looks pretty good: most images are on the main diagonal, which means that they were classified correctly. Notice that the cell on the diagonal on row #5 and column #5 looks slightly darker than the other digits. This could be because the model made more errors on 5s, or because there are simply less 5s in the dataset than the other digits. That's why it's important to normalize the confusion matrix by dividing each value by the total number of images in the corresponding (true) class (i.e., divide by the row's sum). This can be done simply by setting `normalize="true"`. We can also specify `values_format=".0%"` argument to show percentages with no decimals. The following code produces the diagram on the right of Figure 3-9:

```
ConfusionMatrixDisplay.from_predictions(y_train, y_train_pred,
                                        normalize="true",
values_format=".0%")
plt.show()
```



Confusion matrix
5577 0 22 5 8 43 36 6 225 1
0 6400 37 24 4 44 4 7 212 10
27 27 5220 92 73 27 67 36 378 11
22 17 117 5227 2 203 27 40 403 73
12 14 41 9 5182 12 34 27 347 164
27 15 30 168 53 4444 75 14 535 60
30 15 42 3 44 97 5552 3 131 1
21 10 51 30 49 12 3 5684 195 210
17 63 48 86 3 126 25 10 5429 44
25 18 30 64 118 36 1 179 371 5107
True label
Predicted label
0 1 2 3 4 5 6 7 8 9
6000 5000 4000 3000 2000 1000 0
CM normalized by row
94% 0% 0% 0% 0% 1% 1% 0% 4% 0%
0% 95% 1% 0% 0% 1% 0% 0% 3% 0%
0% 0% 88% 2% 1% 0% 1% 1% 6% 0%
0% 0% 2% 85% 0% 3% 0% 1% 7% 1%
0% 0% 1% 0% 89% 0% 1% 0% 6% 3%
0% 0% 1% 3% 1% 82% 1% 0% 10% 1%
1% 0% 1% 0% 1% 2% 94% 0% 2% 0%
0% 0% 1% 0% 1% 0% 0% 91% 3% 3%
0% 1% 1% 1% 0% 2% 0% 0% 93% 1%
0% 0% 1% 1% 2% 1% 0% 3% 6% 86%
True label
Predicted label
0 1 2 3 4 5 6 7 8 9
0.8 0.6 0.4 0.2 0.0

Figure 3-9. Confusion matrix (left) and the same CM normalized by row (right)

Now we can easily see that only 82% of the images of 5s were classified correctly. The most common error the model made with images of 5s was to misclassify them as 8s: this happened for 10% of all 5s. But only 2% of 8s got misclassified as 5s: confusion matrices are generally not symmetrical! If you look carefully, you will notice that many digits have been misclassified as 8s, but this is not immediately obvious on this diagram. If you want to make the errors stand out much more, you can try putting zero weight on the correct predictions. The following code does just that and produces the diagram on the left of Figure 3-10:

```
sample_weight = (y_train_pred != y_train)
ConfusionMatrixDisplay.from_predictions(y_train, y_train_pred,

sample_weight=sample_weight,
                                        normalize="true",
values_format=".0%")
plt.show()
```

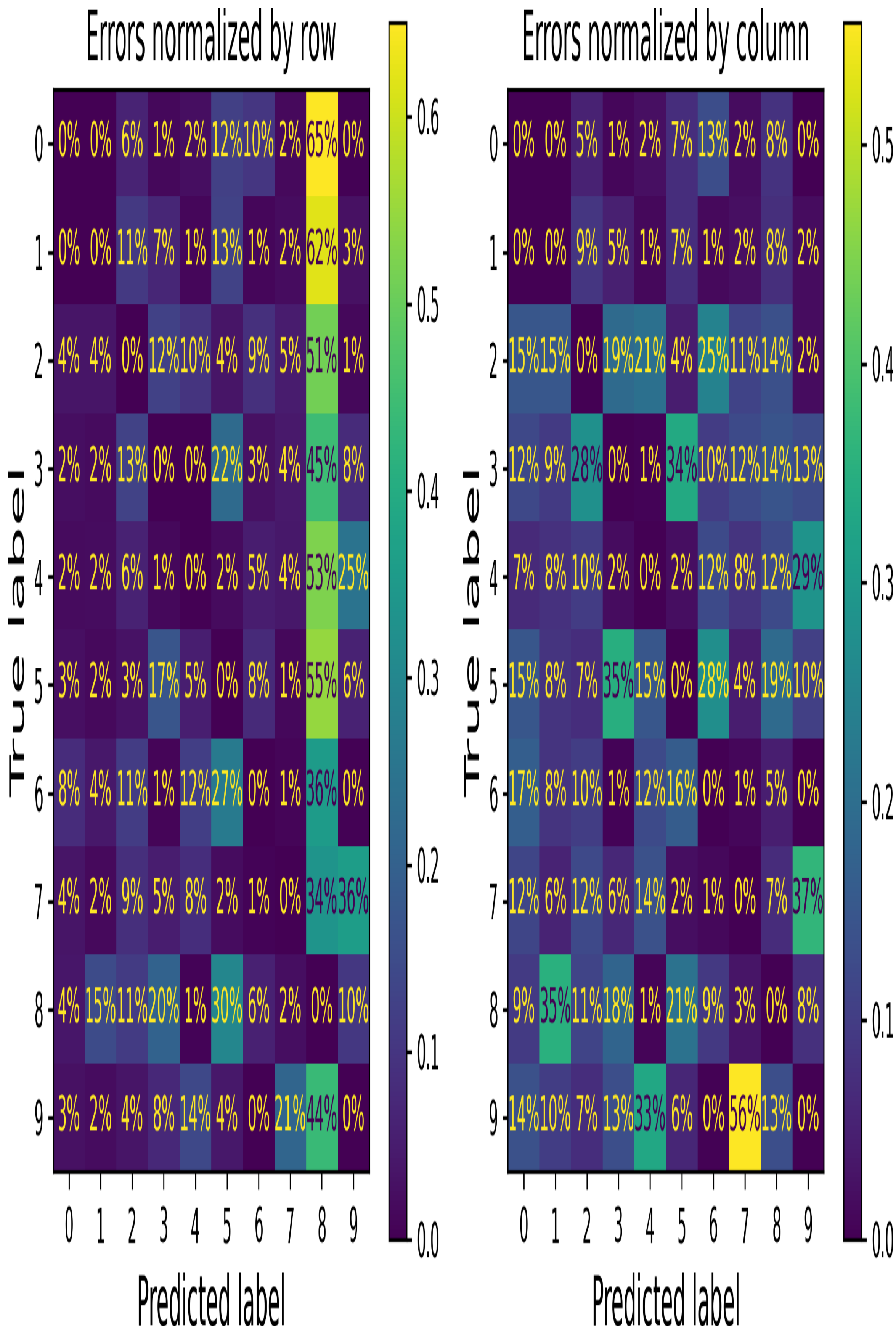

Errors normalized by row
Errors normalized by column
True label
Predicted label

Figure 3-10. Confusion matrix with errors only, normalized by row (left) and by column (right)

Now you can see much more clearly the kinds of errors the classifier makes. The column for class 8 is now really bright, which confirms that many images got misclassified as 8s. In fact this is the most common misclassification for almost all classes. But be careful how you interpret the percentages on this diagram: remember that we've excluded the correct predictions. For example, the 36% in row #7, column #9 does *not* mean that 36% of all images of 7s were misclassified as 9s. It means that 36% of the *errors* the model made on images of 7s were misclassifications as 9s. In reality, only 3% of images of 7s were misclassified as 9s, as you can see in the diagram on the right of Figure 3-9.

It is also possible to normalize the confusion matrix by column rather than by row: if you set `normalize="pred"`, you get the diagram on the right of Figure 3-10. For example, you can see that 56% of misclassified 7s are actually 9s.

Analyzing the confusion matrix often gives you insights into ways to improve your classifier. Looking at these plots, it seems that your efforts should be spent on reducing the false 8s. For example, you could try to gather more training data for digits that look like 8s (but are not) so that the classifier can learn to distinguish them from real 8s. Or you could engineer new features that would help the classifier—for example, writing an algorithm to count the number of closed loops (e.g., 8 has two, 6 has one, 5 has none). Or you could preprocess the images (e.g., using Scikit-Image, Pillow, or OpenCV) to make some patterns, such as closed loops, stand out more.

Analyzing individual errors can also be a good way to gain insights on what your classifier is doing and why it is failing. For example, let's plot examples of 3s and 5s in a confusion matrix style (Figure 3-11):

```
cl_a, cl_b = '3', '5'
X_aa = X_train[(y_train == cl_a) & (y_train_pred == cl_a)]
X_ab = X_train[(y_train == cl_a) & (y_train_pred == cl_b)]
X_ba = X_train[(y_train == cl_b) & (y_train_pred == cl_a)]
X_bb = X_train[(y_train == cl_b) & (y_train_pred == cl_b)]
```

```
[...]  # plot all images in X_aa, X_ab, X_ba, X_bb in a confusion
matrix style
```

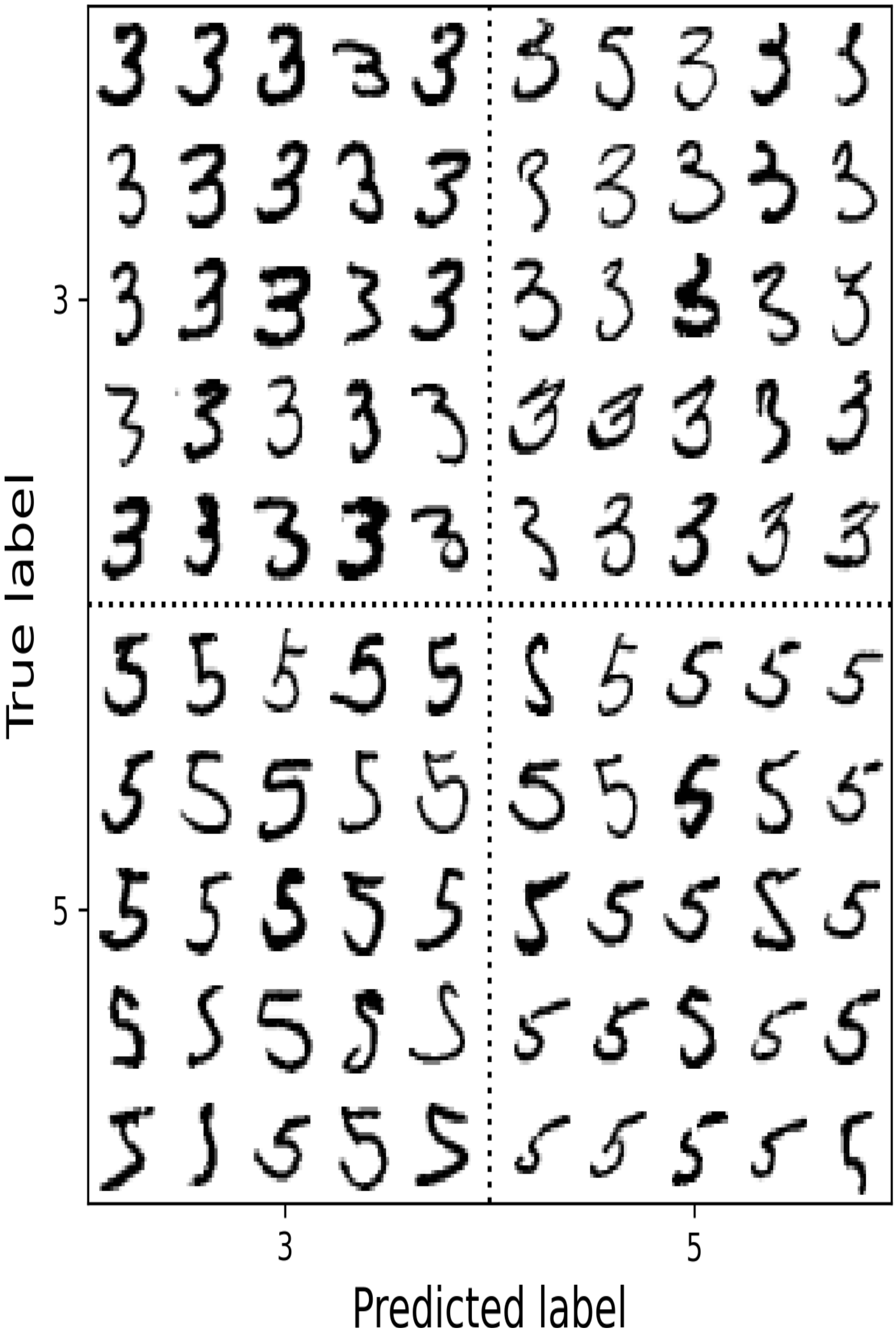

True label
3
5
Predicted label
3
5

Figure 3-11. Some images of 3s and 5s organized like a confusion matrix

As you can see, some of the digits that the classifier gets wrong (i.e., in the bottom-left and top-right blocks) are so badly written that even a human would have trouble classifying them. However, most misclassified images seem like obvious errors to us, and it's hard to understand why the classifier made the mistakes it did. But remember that our brain is a fantastic pattern recognition system, and our visual system does a lot of complex preprocessing before any information even reaches our consciousness, so the fact that it feels simple does not mean that it is. Remember that we used a simple `SGDClassifier`, which is just a linear model: all it does is assign a weight per class to each pixel, and when it sees a new image it just sums up the weighted pixel intensities to get a score for each class. Since 3s and 5s differ only by a few pixels, this model will easily confuse them.

The main difference between 3s and 5s is the position of the small line that joins the top line to the bottom arc. If you draw a 3 with the junction slightly shifted to the left, the classifier might classify it as a 5, and vice versa. In other words, this classifier is quite sensitive to image shifting and rotation. So one way to reduce the 3/5 confusion would be to preprocess the images to ensure that they are well centered and not too rotated. However, this may not be easy at all since it requires predicting the correct rotation of each image. A much simpler approach consists in augmenting the training set with slightly shifted and rotated variants of the training images. This will force the model to learn to be more tolerant to such variations. This is called *data augmentation* (we'll cover this in Chapter 14 and also see exercise 2 at the end of this chapter).

Multilabel Classification

Until now each instance has always been assigned to just one class. In some cases you may want your classifier to output multiple classes for each instance. Consider a face-recognition classifier: what should it do if it recognizes several people in the same picture? It should attach one tag per person it recognizes. Say the classifier has been trained to recognize three faces, Alice, Bob, and Charlie. Then when the classifier is shown a picture of Alice and Charlie, it should output `[True, False, True]` (meaning “Alice yes, Bob no, Charlie yes”). Such a classification system that outputs multiple binary tags is called a *multilabel classification* system.

We won’t go into face recognition just yet, but let’s look at a simpler example, just for illustration purposes:

```
import numpy as np
from sklearn.neighbors import KNeighborsClassifier

y_train_large = (y_train >= '7')
y_train_odd = (y_train.astype('int8') % 2 == 1)
y_multilabel = np.c_[y_train_large, y_train_odd]

knn_clf = KNeighborsClassifier()
knn_clf.fit(X_train, y_multilabel)
```

This code creates a `y_multilabel` array containing two target labels for each digit image: the first indicates whether or not the digit is large (7, 8, or 9), and the second indicates whether or not it is odd. Then the code creates a `KNeighborsClassifier` instance, which supports multilabel classification (not all classifiers do). Then the code trains this model using the multiple targets array. Now you can make a prediction, and notice that it outputs two labels:

```
>>> knn_clf.predict([some_digit])
array([[False,  True]])
```

And it gets it right! The digit 5 is indeed not large (`False`) and odd (`True`).

There are many ways to evaluate a multilabel classifier, and selecting the right metric really depends on your project. One approach is to measure the F_1 score for each individual label (or any other binary classifier metric discussed earlier), then simply compute the average score. The following code computes the average F_1 score across all labels:

```
>>> y_train_knn_pred = cross_val_predict(knn_clf, X_train,
y_multilabel, cv=3)
>>> f1_score(y_multilabel, y_train_knn_pred, average="macro")
0.976410265560605
```

This approach assumes that all labels are equally important, which may not be the case. In particular, if you have many more pictures of Alice than of Bob or Charlie, you may want to give more weight to the classifier's score on pictures of Alice. One simple option is to give each label a weight equal to its *support* (i.e., the number of instances with that target label). To do this, simply set `average="weighted"` when calling the `f1_score()` function.[5]

If you wish to use a classifier that does not natively support multilabel classification, such as `SVC`, one possible strategy is to train one model per label. However, this strategy may have a hard time capturing the dependencies between the labels. For example, a large digit (7, 8, or 9) is twice more likely to be odd than even, but the classifier for the "odd" label does not know what the classifier for the "large" label predicted. To solve this issue, the models can be organized in a chain: when a model makes a prediction, it uses the input features plus all the predictions of the models that come before it in the chain.

Now the good news is that Scikit-Learn has a class called `ChainClassifier` that does just that! By default it will use the true labels for training, feeding each model the appropriate labels depending on their position in the chain. But if you set the `cv` hyperparameter, it will use cross-validation to get "clean" (out-of-sample) predictions from each trained model, for every instance in the training set, and these predictions will then be used to train all the models later in the chain. Here's an example showing how to create and train a `ChainClassifier` using the cross-validation strategy. As earlier, we'll just use the first 2,000 images in the training set to speed things up:

```
from sklearn.multioutput import ClassifierChain
```

```
chain_clf = ClassifierChain(SVC(), cv=3, random_state=42)
chain_clf.fit(X_train[:2000], y_multilabel[:2000])
```

Now we can use this `ChainClassifier` to make predictions:

```
>>> chain_clf.predict([some_digit])
array([[0., 1.]])
```

Multioutput Classification

The last type of classification task we are going to discuss here is called *multioutput–multiclass classification* (or just *multioutput classification*). It is a generalization of multilabel classification where each label can be multiclass (i.e., it can have more than two possible values).

To illustrate this, let's build a system that removes noise from images. It will take as input a noisy digit image, and it will (hopefully) output a clean digit image, represented as an array of pixel intensities, just like the MNIST images. Notice that the classifier's output is multilabel (one label per pixel) and each label can have multiple values (pixel intensity ranges from 0 to 255). It is thus an example of a multioutput classification system.

> **NOTE**
>
> The line between classification and regression is sometimes blurry, such as in this example. Arguably, predicting pixel intensity is more akin to regression than to classification. Moreover, multioutput systems are not limited to classification tasks; you could even have a system that outputs multiple labels per instance, including both class labels and value labels.

Let's start by creating the training and test sets by taking the MNIST images and adding noise to their pixel intensities with NumPy's `randint()` function. The target images will be the original images:

```
np.random.seed(42)  # to make this code example reproducible
noise = np.random.randint(0, 100, (len(X_train), 784))
X_train_mod = X_train + noise
```

```
noise = np.random.randint(0, 100, (len(X_test), 784))
X_test_mod = X_test + noise
y_train_mod = X_train
y_test_mod = X_test
```

Let’s take a peek at the first image from the test set (Figure 3-12). Yes, we’re snooping on the test data, so you should be frowning right now.

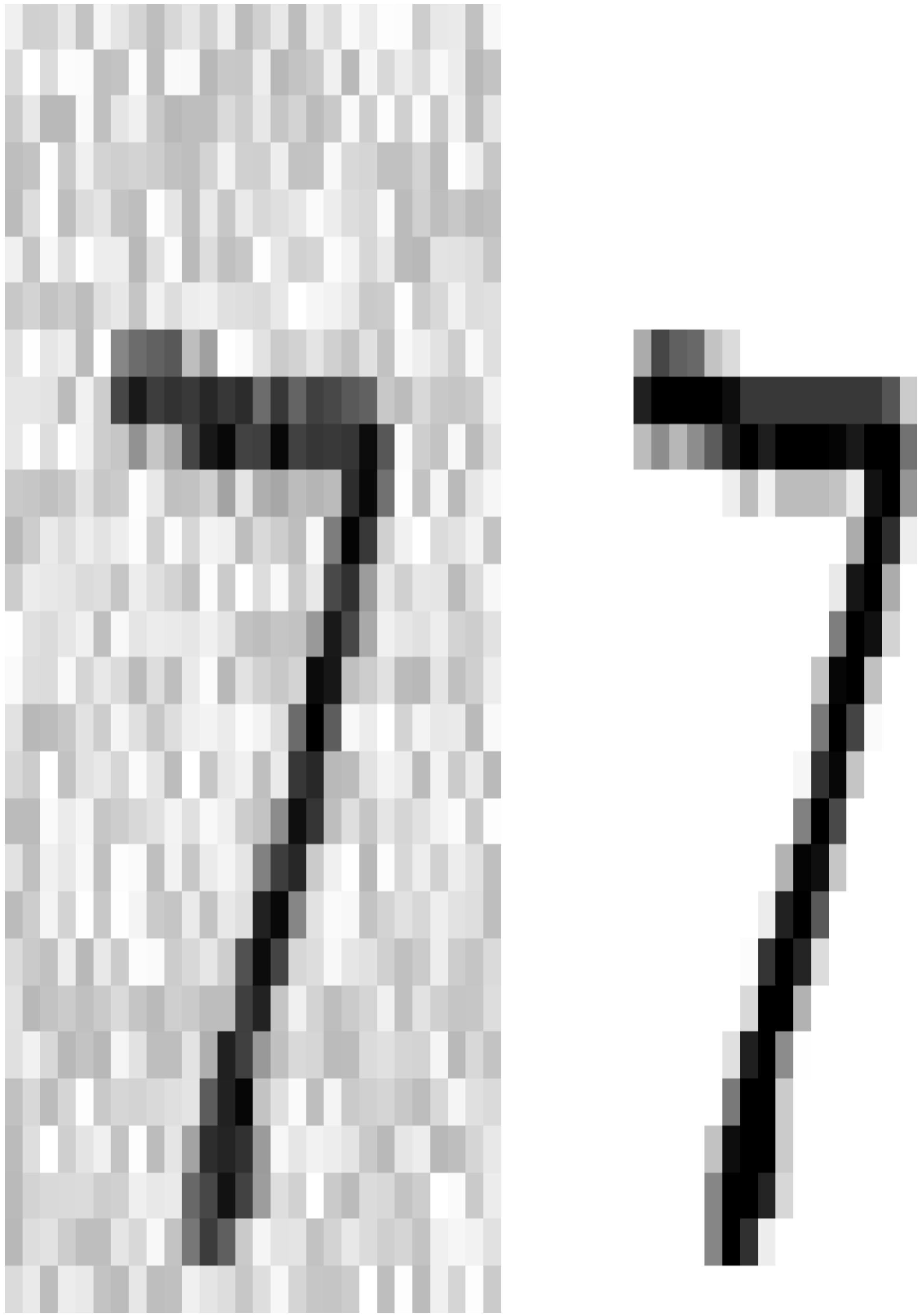


Figure 3-12. A noisy image (left) and the target clean image (right)

On the left is the noisy input image, and on the right is the clean target image. Now let’s train the classifier and make it clean up this image (Figure 3-13):

```
knn_clf = KNeighborsClassifier()
knn_clf.fit(X_train_mod, y_train_mod)
clean_digit = knn_clf.predict([X_test_mod[0]])
plot_digit(clean_digit)
plt.show()
```

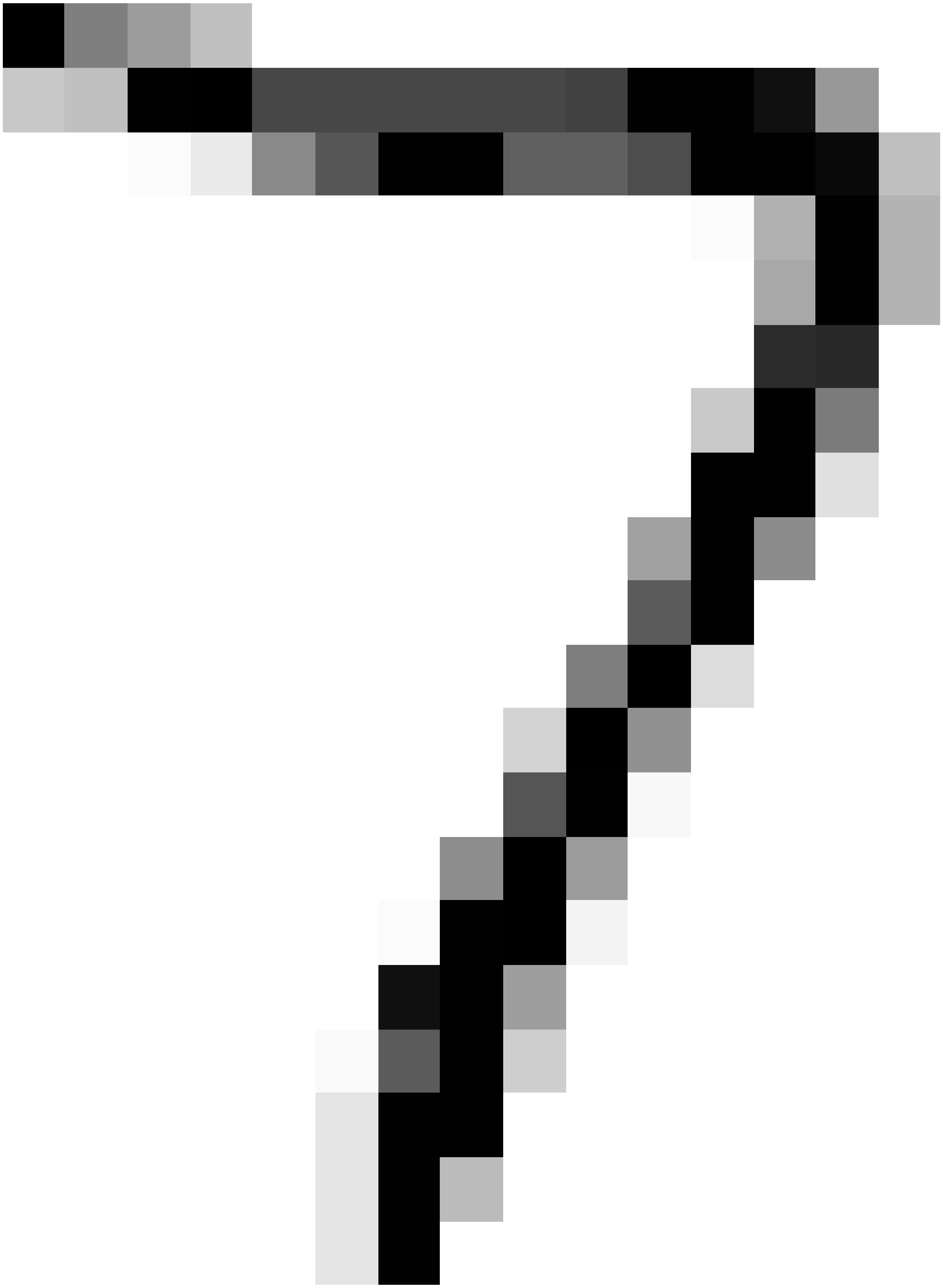


Figure 3-13. The cleaned up image

Looks close enough to the target! Well, this concludes our tour of classification. You now know how to select good metrics for classification tasks, pick the appropriate precision/recall trade-off, compare classifiers, and more generally build good classification systems for a variety of tasks. In the next chapters, we look at how all these Machine Learning models we've been using actually work.

Exercises

1. Try to build a classifier for the MNIST dataset that achieves over 97% accuracy on the test set. Hint: the `KNeighborsClassifier` works quite well for this task; you just need to find good hyperparameter values (try a grid search on the `weights` and `n_neighbors` hyperparameters).

2. Write a function that can shift an MNIST image in any direction (left, right, up, or down) by one pixel.[6] Then, for each image in the training set, create four shifted copies (one per direction) and add them to the training set. Finally, train your best model on this expanded training set and measure its accuracy on the test set. You should observe that your model performs even better now! This technique of artificially growing the training set is called *data augmentation* or *training set expansion*.

3. Tackle the Titanic dataset. A great place to start is on Kaggle. Alternatively, you can download the data from *https://homl.info/titanic.tgz* and unzip this tarball like you did for the housing data in Chapter 2. This will give you two CSV files: *train.csv* and *test.csv* which you can load using `pandas.read_csv()`. The goal is to train a classifier that can predict the `Survived` column based on the other columns.

4. Build a spam classifier (a more challenging exercise):

- Download examples of spam and ham from Apache SpamAssassin's public datasets.
- Unzip the datasets and familiarize yourself with the data format.
- Split the datasets into a training set and a test set.
- Write a data preparation pipeline to convert each email into a feature vector. Your preparation pipeline should transform an email into a (sparse) vector that indicates the presence or absence of each possible word. For example, if all emails only ever contain four words, "Hello," "how," "are," "you," then the email "Hello you Hello Hello you" would be converted into a vector [1, 0, 0, 1] (meaning ["Hello" is present, "how" is absent, "are" is absent, "you" is present]), or [3, 0, 0, 2] if you prefer to count the number of occurrences of each word.

  You may want to add hyperparameters to your preparation pipeline to control whether or not to strip off email headers, convert each email to lowercase, remove punctuation, replace all URLs with "URL," replace all numbers with "NUMBER," or even perform *stemming* (i.e., trim off word endings; there are Python libraries available to do this).

  Finally, try out several classifiers and see if you can build a great spam classifier, with both high recall and high precision.

Solutions to these exercises are available at the end of this chapter's notebook, at *https://homl.info/colab3*.

---

1 By default Scikit-Learn caches downloaded datasets in a directory called *scikit_learn_data* in your home directory.

2 Datasets returned by `fetch_openml()` are not always shuffled or split.

3 Shuffling may be a bad idea in some contexts—for example, if you are working on time series data (such as stock market prices or weather conditions). We will explore this in Chapter 15.

4 Scikit-Learn classifiers always have either a `decision_function()` method or a `predict_proba()` method, or sometimes both.

5 Scikit-Learn offers a few other averaging options and multilabel classifier metrics; see the documentation for more details.

6 You can use the `shift()` function from the `scipy.ndimage.interpolation` module. For example, `shift(image, [2, 1], cval=0)` shifts the image two pixels down and one pixel to the right.

Chapter 4. Training Models

A NOTE FOR EARLY RELEASE READERS

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.

This will be the 4th chapter of the final book. Notebooks are available on GitHub at *https://github.com/ageron/handson-ml3*. Datasets are available at *https://github.com/ageron/data*.

If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the editoor at ntache@oreilly.com.

So far we have treated Machine Learning models and their training algorithms mostly like black boxes. If you went through some of the exercises in the previous chapters, you may have been surprised by how much you can get done without knowing anything about what's under the hood: you optimized a regression system, you improved a digit image classifier, and you even built a spam classifier from scratch, all this without knowing how they actually work. Indeed, in many situations you don't really need to know the implementation details.

However, having a good understanding of how things work can help you quickly home in on the appropriate model, the right training algorithm to use, and a good set of hyperparameters for your task. Understanding what's under the hood will also help you debug issues and perform error analysis more efficiently. Lastly, most of the topics discussed in this chapter will be essential in understanding, building, and training neural networks (discussed in Part II of this book).

In this chapter we will start by looking at the Linear Regression model, one of the simplest models there is. We will discuss two very different ways to train it:

- Using a "closed-form" equation that directly computes the model parameters that best fit the model to the training set (i.e., the model parameters that minimize the cost function over the training set).
- Using an iterative optimization approach called Gradient Descent (GD) that gradually tweaks the model parameters to minimize the cost function over the training set, eventually converging to the same set of parameters as the first method. We will look at a few variants of Gradient Descent that we will use again and again when we study neural networks in Part II: Batch GD, Mini-batch GD, and Stochastic GD.

Next we will look at Polynomial Regression, a more complex model that can fit nonlinear datasets. Since this model has more parameters than Linear Regression, it is more prone to overfitting the training data, so we will look at how to detect whether or not this is the case using learning curves, and then we will look at several regularization techniques that can reduce the risk of overfitting the training set.

Finally, we will look at two more models that are commonly used for classification tasks: Logistic Regression and Softmax Regression.

WARNING

There will be quite a few math equations in this chapter, using basic notions of linear algebra and calculus. To understand these equations, you will need to know what vectors and matrices are; how to transpose them, multiply them, and inverse them; and what partial derivatives are. If you are unfamiliar with these concepts, please go through the linear algebra and calculus introductory tutorials available as Jupyter notebooks in the online supplemental material. For those who are truly allergic to mathematics, you should still go through this chapter and simply skip the equations; hopefully, the text will be sufficient to help you understand most of the concepts.

Linear Regression

In Chapter 1 we looked at a simple regression model of life satisfaction: *life_satisfaction* = $\theta_0 + \theta_1 \times$ *GDP_per_capita*.

This model is just a linear function of the input feature `GDP_per_capita`. θ_0 and θ_1 are the model's parameters.

More generally, a linear model makes a prediction by simply computing a weighted sum of the input features, plus a constant called the *bias term* (also called the *intercept term*), as shown in Equation 4-1.

Equation 4-1. Linear Regression model prediction

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$$

In this equation:

- $\hat{y}$ is the predicted value.
- n is the number of features.
- x_i is the i^{th} feature value.
- θ_j is the j^{th} model parameter, including the bias term θ_0 and the feature weights $\theta_1, \theta_2, \cdots, \theta_n$.

This can be written much more concisely using a vectorized form, as shown in Equation 4-2.

Equation 4-2. Linear Regression model prediction (vectorized form)

$$\hat{y} = h_{\boldsymbol{\theta}}\left(\mathbf{x}\right) = \boldsymbol{\theta} \cdot \mathbf{x}$$

In this equation:

- $h_{\boldsymbol{\theta}}$ is the hypothesis function, using the model parameters $\boldsymbol{\theta}$.
- $\boldsymbol{\theta}$ is the model's *parameter vector*, containing the bias term θ_0 and the feature weights θ_1 to θ_n.
- $\mathbf{x}$ is the instance's *feature vector*, containing x_0 to x_n, with x_0 always equal to 1.
- $\boldsymbol{\theta} \cdot \mathbf{x}$ is the dot product of the vectors $\boldsymbol{\theta}$ and $\mathbf{x}$, which is equal to $\theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + ... + \theta_n x_n$.

> **NOTE**
>
> In Machine Learning, vectors are often represented as *column vectors*, which are 2D arrays with a single column. If $\boldsymbol{\theta}$ and $\mathbf{x}$ are column vectors, then the prediction is $\hat{y} = \boldsymbol{\theta}^{\intercal}\mathbf{x}$, where $\boldsymbol{\theta}^{\intercal}$ is the *transpose* of $\boldsymbol{\theta}$ (a row vector instead of a column vector) and $\boldsymbol{\theta}^{\intercal}\mathbf{x}$ is the matrix multiplication of $\boldsymbol{\theta}^{\intercal}$ and $\mathbf{x}$. It is of course the same prediction, except that it is now represented as a single-cell matrix rather than a scalar value. In this book I will use this notation to avoid switching between dot products and matrix multiplications.

OK, that's the Linear Regression model—but how do we train it? Well, recall that training a model means setting its parameters so that the model best fits the training set. For this purpose, we first need a measure of how well (or poorly) the model fits the training data. In Chapter 2 we saw that the most common performance measure of a regression model is the Root Mean Square Error (RMSE) (Equation 2-1). Therefore, to train a Linear Regression model, we need to find the value of $\boldsymbol{\theta}$ that minimizes the RMSE. In practice, it is simpler to minimize the mean squared error (MSE) than the RMSE, and it leads to the same result (because the value that minimizes a positive function also minimizes its square root).

WARNING

Learning algorithms will often optimize a different loss function during training than the performance measure used to evaluate the final model. This is generally because the function is easier to optimize and/or because it has extra terms needed during training only (e.g., for regularization). A good performance metric is as close as possible to the final business objective. A good training loss is easy to optimize and strongly correlated with the metric. For example, classifiers are often trained using a cost function such as the log loss (as we will see later in this chapter) but evaluated using precision/recall. The log loss is easy to minimize, and doing so will usually improve precision/recall.

The MSE of a Linear Regression hypothesis $h_{\boldsymbol{\theta}}$ on a training set $\mathbf{X}$ is calculated using Equation 4-3.

Equation 4-3. MSE cost function for a Linear Regression model

$$\text{MSE}\left(\mathbf{X}, h_{\boldsymbol{\theta}}\right) = \frac{1}{m}\sum_{i=1}^{m}\left(\boldsymbol{\theta}^{\intercal}\mathbf{x}^{(i)} - y^{(i)}\right)^2$$

Most of these notations were presented in Chapter 2 (see "Notations"). The only difference is that we write $h_{\boldsymbol{\theta}}$ instead of just h to make it clear that the model is parametrized by the vector $\boldsymbol{\theta}$. To simplify notations, we will just write MSE($\boldsymbol{\theta}$) instead of MSE($\mathbf{X}$, $h_{\boldsymbol{\theta}}$).

The Normal Equation

To find the value of $\boldsymbol{\theta}$ that minimizes the MSE, there exists a *closed-form solution*—in other words, a mathematical equation that gives the result directly. This is called the *Normal Equation* (Equation 4-4).

Equation 4-4. Normal Equation

$$\widehat{\boldsymbol{\theta}} = \left(\mathbf{X}^{\intercal}\mathbf{X}\right)^{-1}\ \mathbf{X}^{\intercal}\ \mathbf{y}$$

In this equation:

- $\widehat{\boldsymbol{\theta}}$ is the value of $\boldsymbol{\theta}$ that minimizes the cost function.
- $\mathbf{y}$ is the vector of target values containing $y^{(1)}$ to $y^{(m)}$.

Let's generate some linear-looking data to test this equation on (Figure 4-1):

```python
import numpy as np

np.random.seed(42)  # to make this code example reproducible
m = 100  # number of instances
X = 2 * np.random.rand(m, 1)  # column vector
y = 4 + 3 * X + np.random.randn(m, 1)  # column vector
```

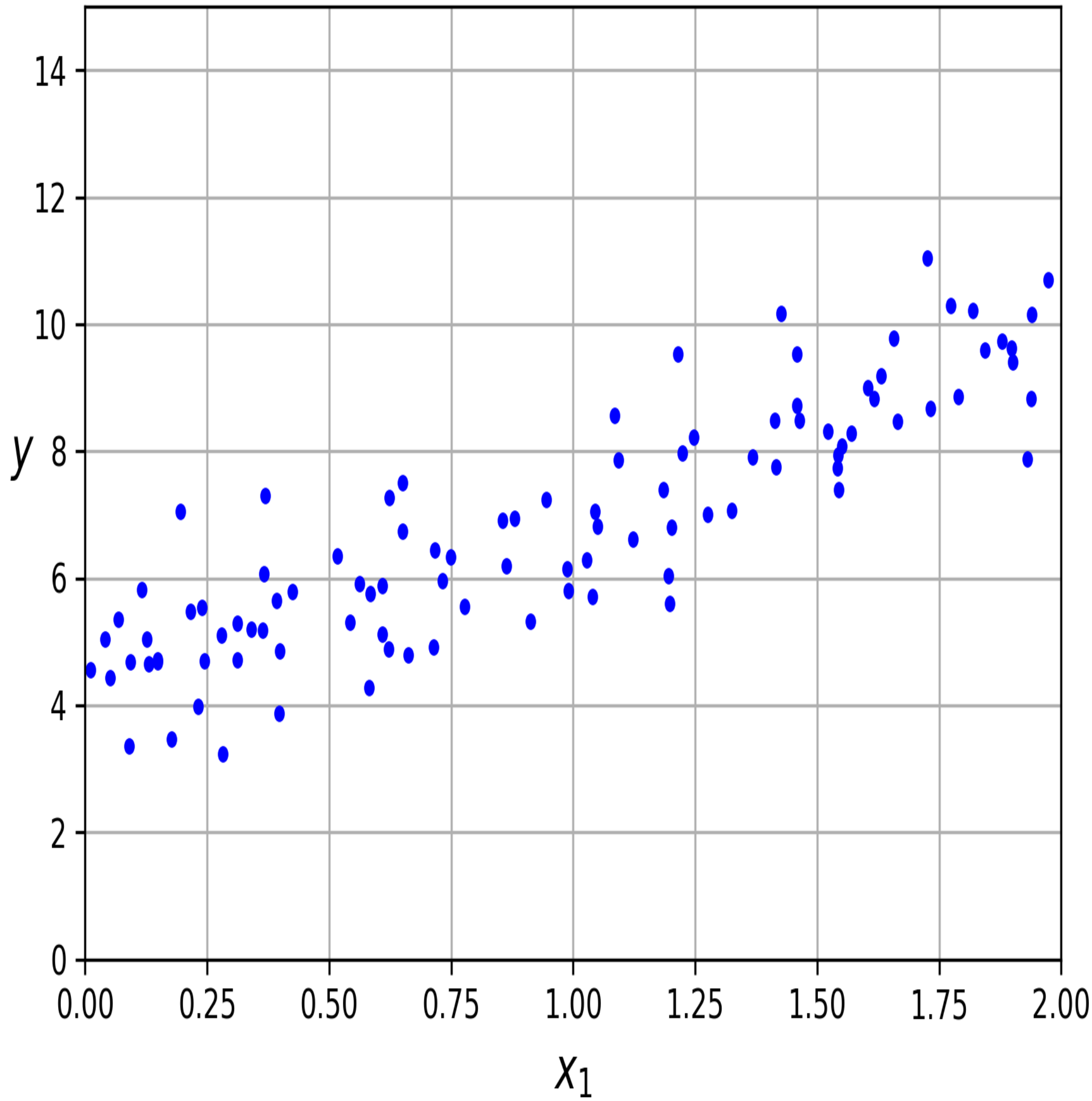


Figure 4-1. Randomly generated linear dataset

Now let's compute $\widehat{\boldsymbol{\theta}}$ using the Normal Equation. We will use the `inv()` function from NumPy's linear algebra module (`np.linalg`) to compute the inverse of a matrix, and the `dot()` method for matrix multiplication:

```
from sklearn.preprocessing import add_dummy_feature

X_b = add_dummy_feature(X)  # add x0 = 1 to each instance
theta_best = np.linalg.inv(X_b.T @ X_b) @ X_b.T @ y
```

> **NOTE**
>
> The `@` operator performs matrix multiplication. If `A` and `B` are NumPy arrays, then `A @ B` is equivalent to `np.matmul(A, B)`. Many other libraries like TensorFlow, PyTorch, or Jax, support the `@` operator as well. However, you cannot use `@` on pure Python arrays (i.e., lists of lists).

The function that we used to generate the data is $y = 4 + 3x_1$ + Gaussian noise. Let's see what the equation found:

```
>>> theta_best
array([[4.21509616],
       [2.77011339]])
```

We would have hoped for $\theta_0 = 4$ and $\theta_1 = 3$ instead of $\theta_0 = 4.215$ and $\theta_1 = 2.770$. Close enough, but the noise made it impossible to recover the exact parameters of the original function. The smaller and noisier the dataset, the harder it gets.

Now we can make predictions using $\widehat{\boldsymbol{\theta}}$:

```
>>> X_new = np.array([[0], [2]])
>>> X_new_b = add_dummy_feature(X_new)  # add x0 = 1 to each instance
>>> y_predict = X_new_b @ theta_best
>>> y_predict
array([[4.21509616],
       [9.75532293]])
```

Let's plot this model's predictions (Figure 4-2):

```
import matplotlib.pyplot as plt

plt.plot(X_new, y_predict, "r-", label="Predictions")
plt.plot(X, y, "b.")
[...]  # beautify the figure: add labels, axis, grid and legend
plt.show()
```

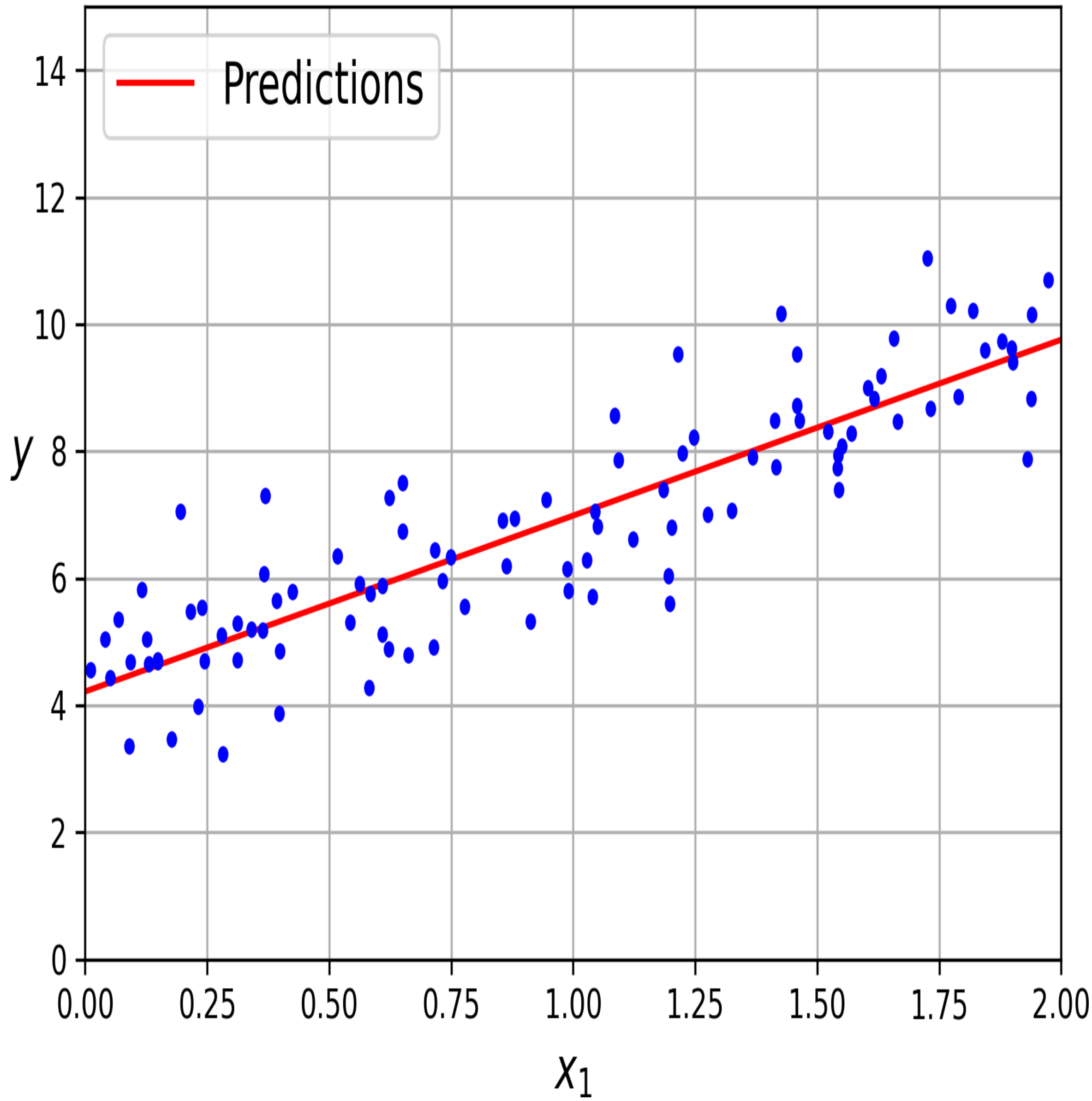


Figure 4-2. Linear Regression model predictions

Performing Linear Regression using Scikit-Learn is relatively straightforward:

```
>>> from sklearn.linear_model import LinearRegression
>>> lin_reg = LinearRegression()
>>> lin_reg.fit(X, y)
>>> lin_reg.intercept_, lin_reg.coef_
(array([4.21509616]), array([[2.77011339]]))
>>> lin_reg.predict(X_new)
array([[4.21509616],
       [9.75532293]])
```

Notice that Scikit-Learn separates the bias term (`intercept_`) from the feature weights (`coef_`). The `LinearRegression` class is based on the `scipy.linalg.lstsq()` function (the name stands for "least squares"), which you could call directly:

```
>>> theta_best_svd, residuals, rank, s = np.linalg.lstsq(X_b, y, rcond=1e-6)
>>> theta_best_svd
array([[4.21509616],
       [2.77011339]])
```

This function computes $\widehat{\boldsymbol{\theta}} = \mathbf{X}^{+}\mathbf{y}$, where $\mathbf{X}^{+}$ is the *pseudoinverse* of $\mathbf{X}$ (specifically, the Moore-Penrose inverse). You can use `np.linalg.pinv()` to compute the pseudoinverse directly:

```
>>> np.linalg.pinv(X_b) @ y
array([[4.21509616],
       [2.77011339]])
```

The pseudoinverse itself is computed using a standard matrix factorization technique called *Singular Value Decomposition* (SVD) that can decompose the training set matrix $\mathbf{X}$ into the matrix multiplication of three matrices $\mathbf{U}\ \boldsymbol{\Sigma}\ \mathbf{V}^{\intercal}$ (see `numpy.linalg.svd()`). The pseudoinverse is computed as $\mathbf{X}^{+} = \mathbf{V}\boldsymbol{\Sigma}^{+}\mathbf{U}^{\intercal}$. To compute the matrix $\boldsymbol{\Sigma}^{+}$, the algorithm takes $\boldsymbol{\Sigma}$ and sets to zero all values smaller than a tiny threshold value, then it replaces all the nonzero values with their inverse, and finally it transposes the resulting matrix. This approach is more efficient than computing the Normal Equation, plus it handles edge cases nicely: indeed, the Normal Equation may not work if the matrix $\mathbf{X}^{\intercal}\mathbf{X}$ is not invertible (i.e., singular), such as if $m < n$ or if some features are redundant, but the pseudoinverse is always defined.

Computational Complexity

The Normal Equation computes the inverse of $\mathbf{X}^{\intercal}\ \mathbf{X}$, which is an $(n + 1) \times (n + 1)$ matrix (where n is the number of features). The *computational complexity* of inverting such a matrix is typically about $O(n^{2.4})$ to $O(n^3)$, depending on the implementation. In other words, if you double the number of features, you multiply the computation time by roughly $2^{2.4} = 5.3$ to $2^3 = 8$.

The SVD approach used by Scikit-Learn's `LinearRegression` class is about $O(n^2)$. If you double the number of features, you multiply the computation time by roughly 4.

> **WARNING**
>
> Both the Normal Equation and the SVD approach get very slow when the number of features grows large (e.g., 100,000). On the positive side, both are linear with regard to the number of instances in the training set (they are O(m_)), so they handle large training sets efficiently, provided they can fit in memory.

Also, once you have trained your Linear Regression model (using the Normal Equation or any other algorithm), predictions are very fast: the computational complexity is linear with regard to both the number of instances you want to make predictions on and the number of features. In other words, making predictions on twice as many instances (or twice as many features) will take roughly twice as much time.

Now we will look at a very different way to train a Linear Regression model, which is better suited for cases where there are a large number of features or too many training instances to fit in memory.

Gradient Descent

Gradient Descent is a generic optimization algorithm capable of finding optimal solutions to a wide range of problems. The general idea of Gradient Descent is to tweak parameters iteratively in order to minimize a cost function.

Suppose you are lost in the mountains in a dense fog, and you can only feel the slope of the ground below your feet. A good strategy to get to the bottom of the valley quickly is to go downhill in the direction of the steepest slope. This is exactly what Gradient Descent does: it measures the local gradient of the error function with regard to the parameter vector **θ**, and it goes in the direction of descending gradient. Once the gradient is zero, you have reached a minimum!

In practice, you start by filling **θ** with random values (this is called *random initialization*). Then you improve it gradually, taking one baby step at a time, each step attempting to decrease the cost function (e.g., the MSE), until the algorithm *converges* to a minimum (see Figure 4-3).

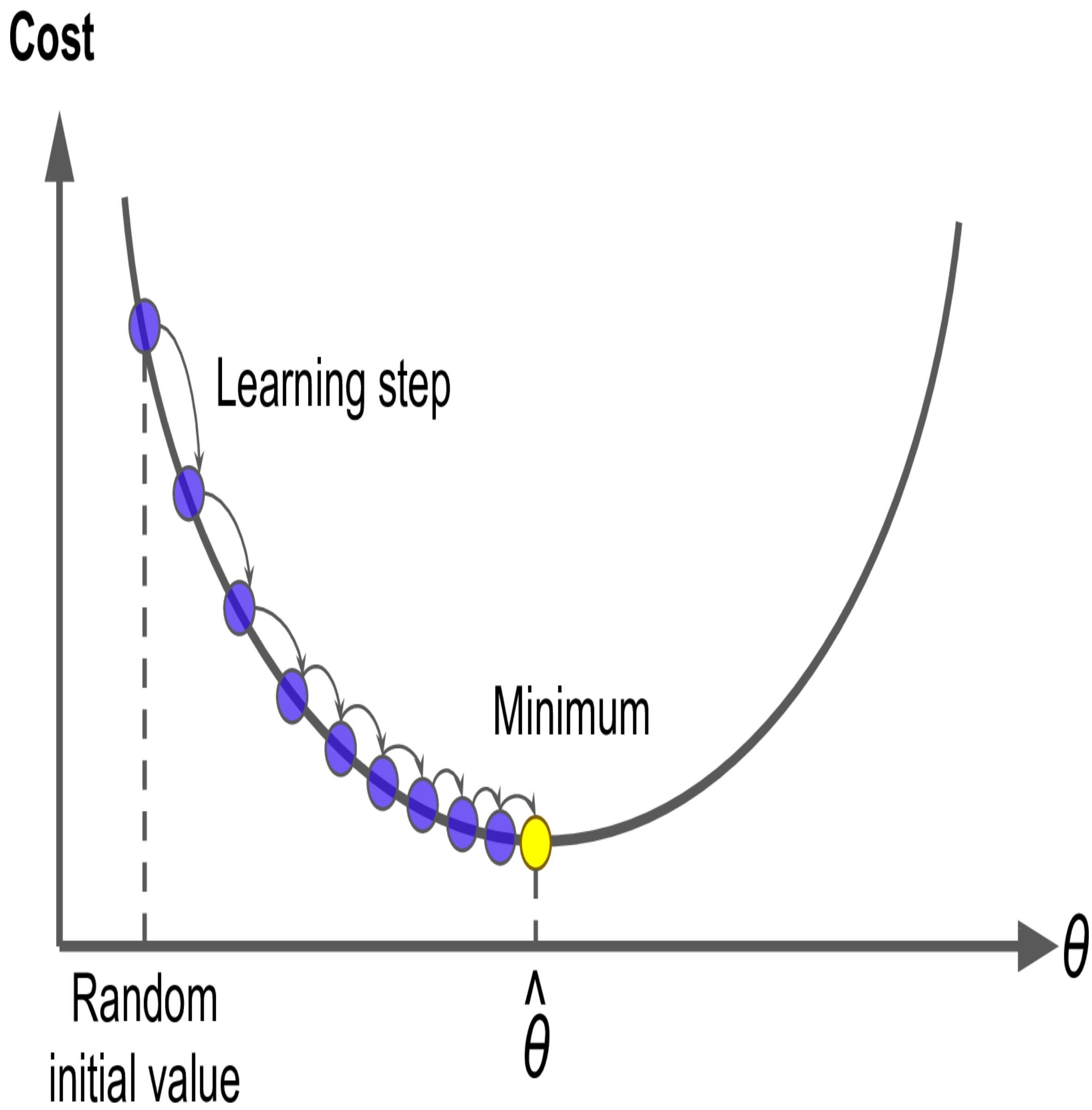


Figure 4-3. In this depiction of Gradient Descent, the model parameters are initialized randomly and get tweaked repeatedly to minimize the cost function; the learning step size is proportional to the slope of the cost function, so the steps gradually get smaller as the cost approaches the minimum

An important parameter in Gradient Descent is the size of the steps, determined by the *learning rate* hyperparameter. If the learning rate is too small, then the algorithm will have to go through many iterations to converge, which will take a long time (see Figure 4-4).

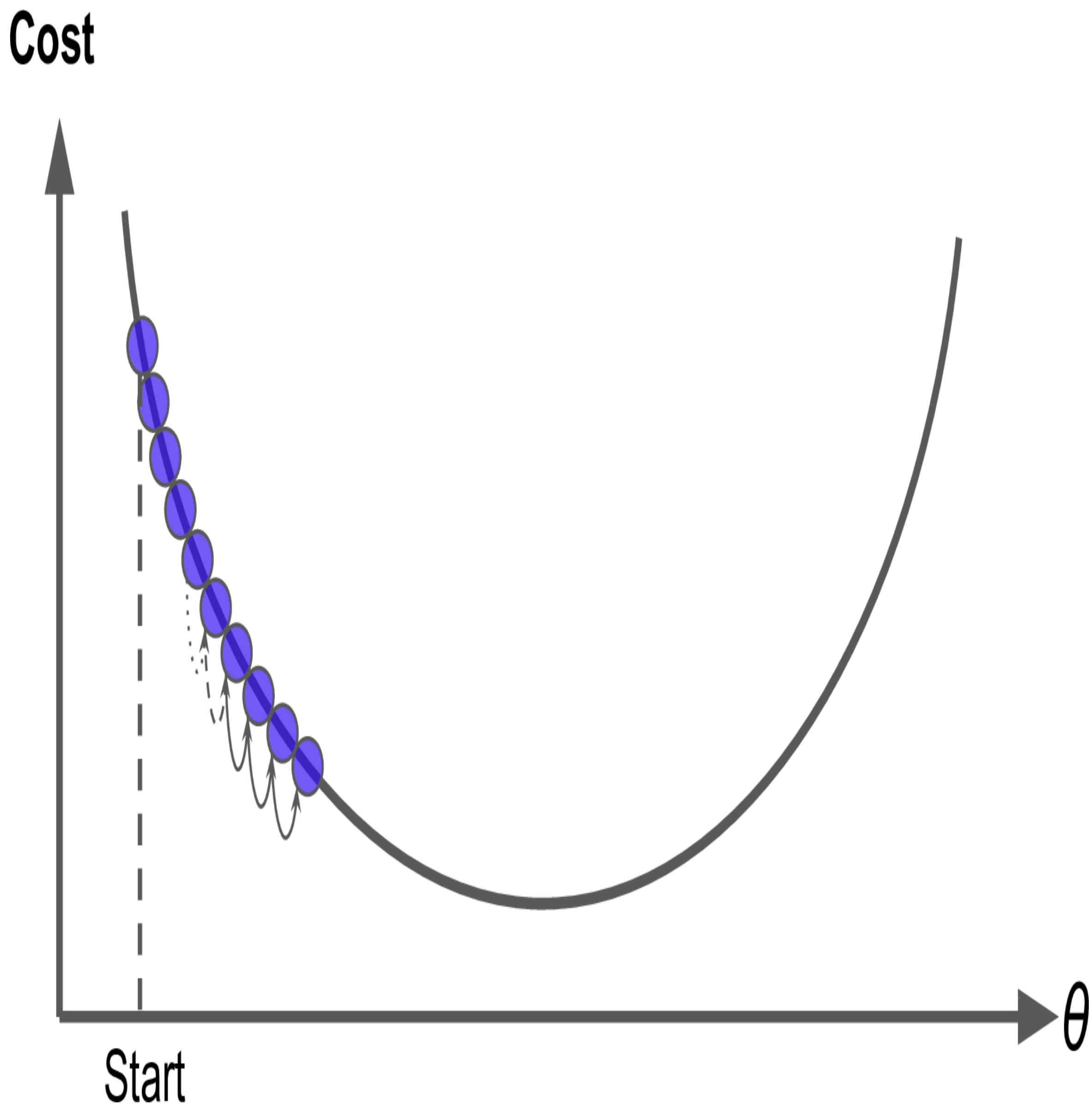


Figure 4-4. The learning rate is too small

On the other hand, if the learning rate is too high, you might jump across the valley and end up on the other side, possibly even higher up than you were before. This might make the algorithm diverge, with larger and larger values, failing to find a good solution (see Figure 4-5).

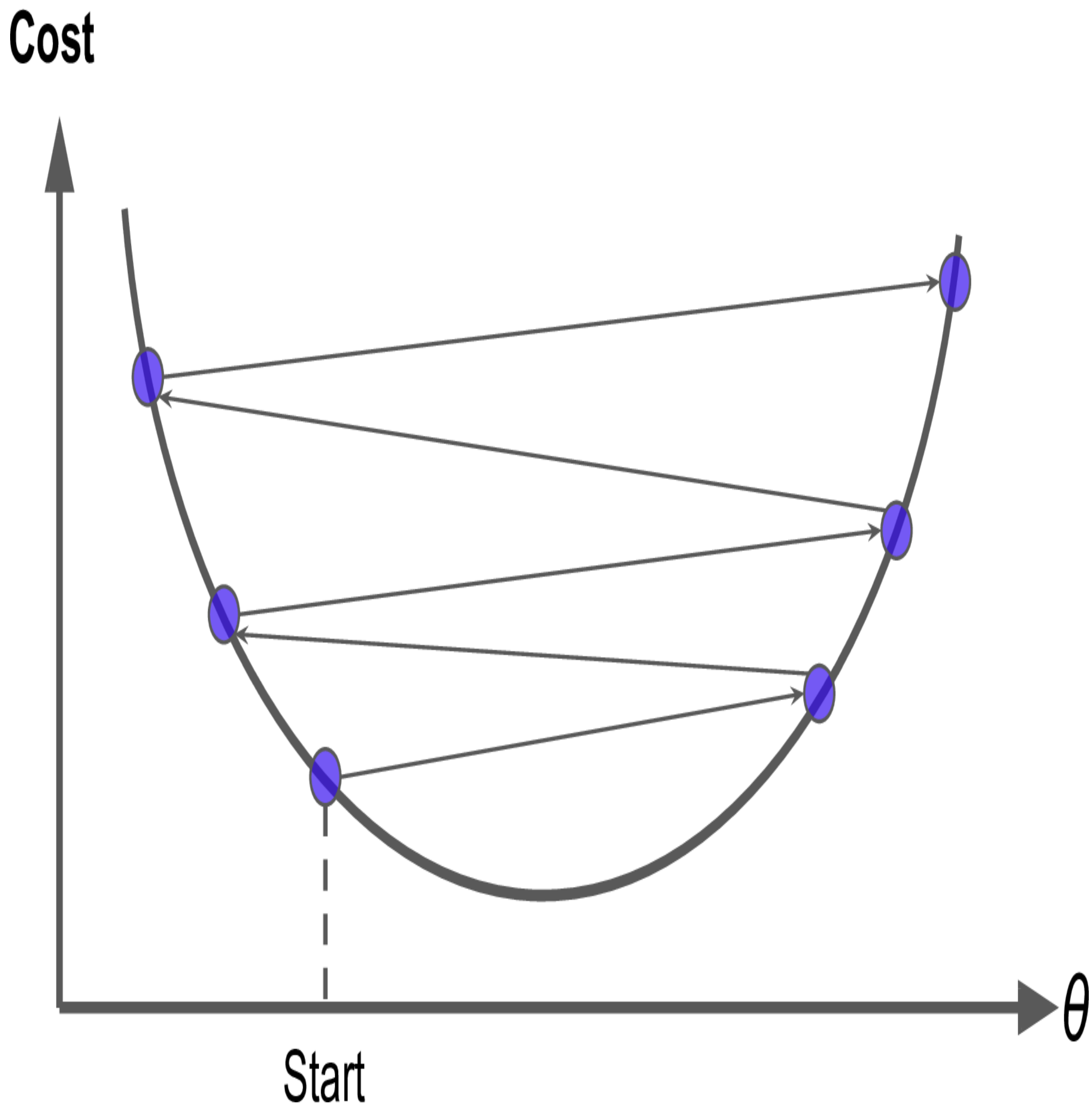


Figure 4-5. The learning rate is too large

Finally, not all cost functions look like nice, regular bowls. There may be holes, ridges, plateaus, and all sorts of irregular terrains, making convergence to the minimum difficult. Figure 4-6 shows the two main challenges with Gradient Descent. If the random initialization starts the algorithm on the left, then it will converge to a *local minimum*, which is not as good as the *global minimum*. If it starts on the right, then it will take a very long time to cross the plateau. And if you stop too early, you will never reach the global minimum.

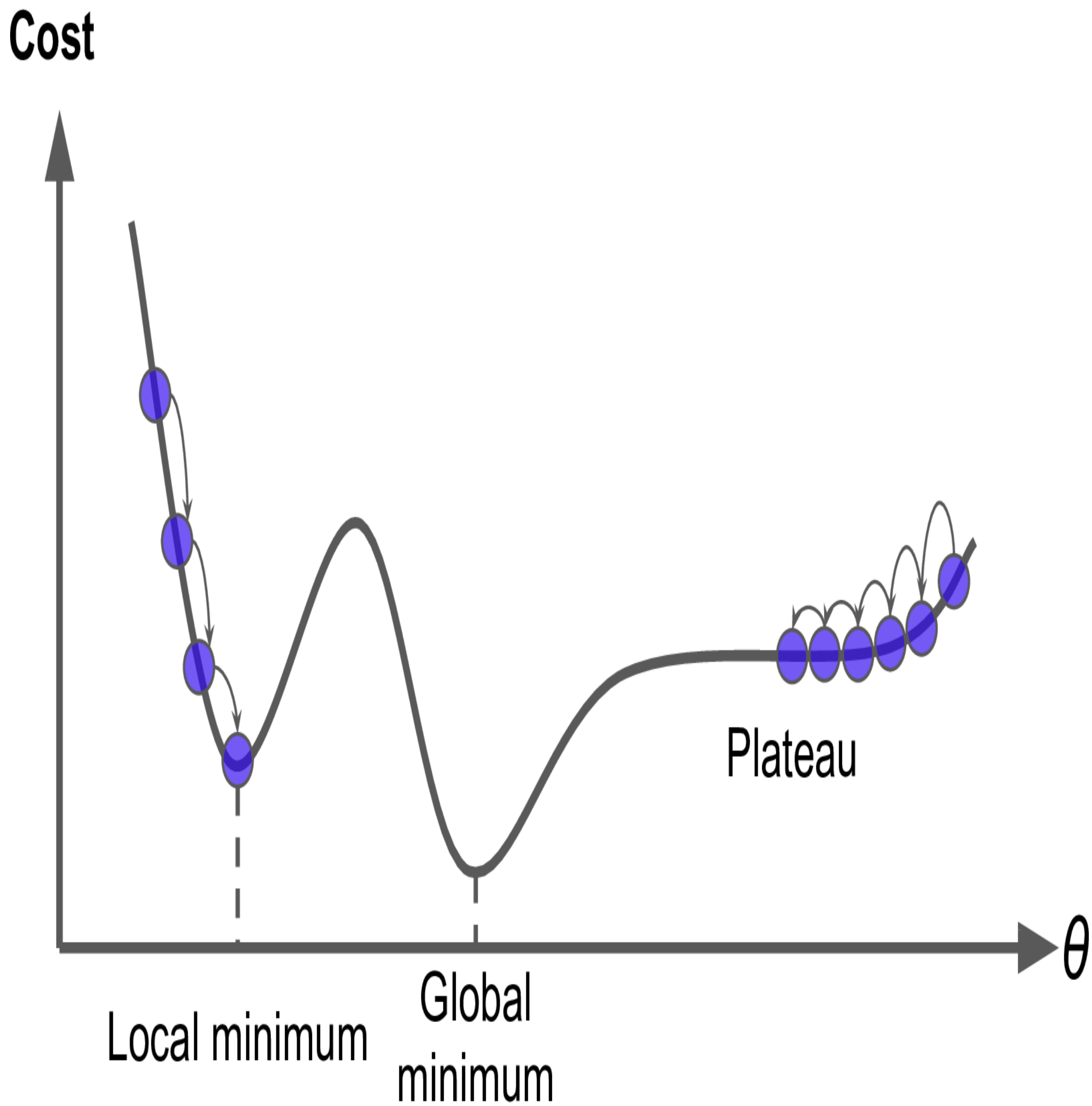


Figure 4-6. Gradient Descent pitfalls

Fortunately, the MSE cost function for a Linear Regression model happens to be a *convex function*, which means that if you pick any two points on the curve, the line segment joining them is never below the curve. This implies that there are no local minima, just one global minimum. It is also a continuous function with a slope that never changes abruptly.[1] These two facts have a great consequence: Gradient Descent is guaranteed to approach arbitrarily close the global minimum (if you wait long enough and if the learning rate is not too high).

In fact, the cost function has the shape of a bowl, but it can be an elongated bowl if the features have very different scales. Figure 4-7 shows Gradient Descent on a training set where features 1 and 2 have the same scale (on the left), and on a training set where feature 1 has much smaller values than feature 2 (on the right).[2]

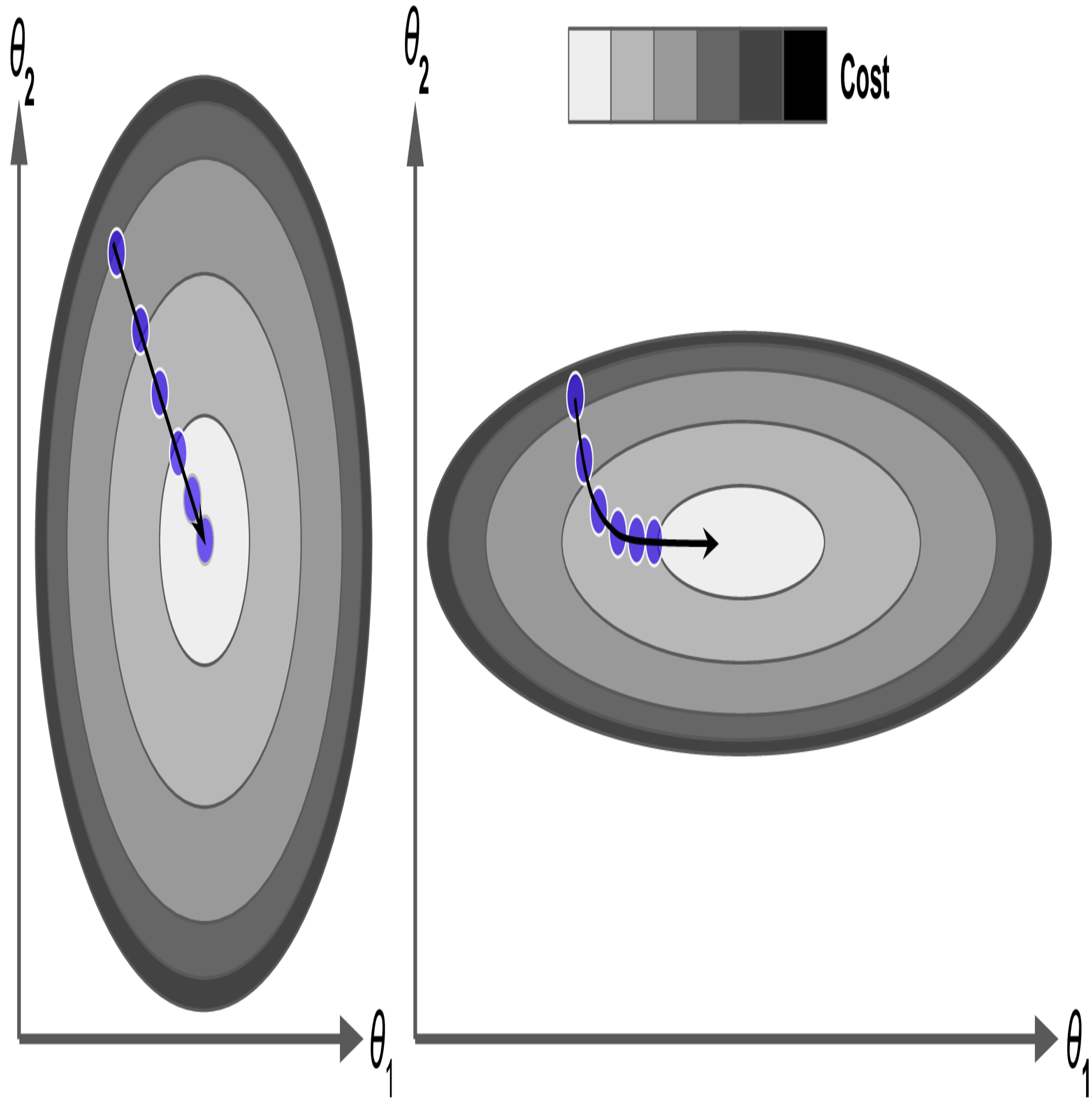


Figure 4-7. Gradient Descent with (left) and without (right) feature scaling

As you can see, on the left the Gradient Descent algorithm goes straight toward the minimum, thereby reaching it quickly, whereas on the right it first goes in a direction almost orthogonal to the direction of the global minimum, and it ends with a long march down an almost flat valley. It will eventually reach the minimum, but it will take a long time.

> **WARNING**
>
> When using Gradient Descent, you should ensure that all features have a similar scale (e.g., using Scikit-Learn's `StandardScaler` class), or else it will take much longer to converge.

This diagram also illustrates the fact that training a model means searching for a combination of model parameters that minimizes a cost function (over the training set). It is a search in the model's *parameter space*: the more parameters a model has, the more dimensions this space has, and the harder the search is: searching for a needle in a 300-dimensional haystack is much trickier than in 3 dimensions. Fortunately, since the cost function is convex in the case of Linear Regression, the needle is simply at the bottom of the bowl.

Batch Gradient Descent

To implement Gradient Descent, you need to compute the gradient of the cost function with regard to each model parameter θ_j. In other words, you need to calculate how much the cost function will change if you change θ_j just a little bit. This is called a *partial derivative*. It is like asking "What is the slope of the mountain under my feet if I face east?" and then asking the same question facing north (and so on for all other dimensions, if you can imagine a universe with more than three dimensions). Equation 4-5 computes the partial derivative of the MSE with regard to parameter θ_j, noted $\partial \text{MSE}(\boldsymbol{\theta}) / \partial\theta_j$.

Equation 4-5. Partial derivatives of the cost function

$$\frac{\partial}{\partial \theta_j} \text{MSE}\left(\boldsymbol{\theta}\right) = \frac{2}{m} \sum_{i=1}^{m} \left(\boldsymbol{\theta}^\intercal \mathbf{x}^{(i)} - y^{(i)}\right) x_j^{(i)}$$

Instead of computing these partial derivatives individually, you can use Equation 4-6 to compute them all in one go. The gradient vector, noted $\nabla_{\boldsymbol{\theta}}\text{MSE}(\boldsymbol{\theta})$, contains all the partial derivatives of the cost function (one for each model parameter).

Equation 4-6. Gradient vector of the cost function

$$\nabla_{\boldsymbol{\theta}} \text{MSE}\left(\boldsymbol{\theta}\right) = \begin{pmatrix} \frac{\partial}{\partial \theta_0} \text{MSE}\left(\boldsymbol{\theta}\right) \\ \frac{\partial}{\partial \theta_1} \text{MSE}\left(\boldsymbol{\theta}\right) \\ \vdots \\ \frac{\partial}{\partial \theta_n} \text{MSE}\left(\boldsymbol{\theta}\right) \end{pmatrix} = \frac{2}{m} \mathbf{X}^\intercal \left(\mathbf{X}\boldsymbol{\theta} - \mathbf{y}\right)$$

> **WARNING**
>
> Notice that this formula involves calculations over the full training set **X**, at each Gradient Descent step! This is why the algorithm is called *Batch Gradient Descent*: it uses the whole batch of training data at every step (actually, *Full Gradient Descent* would probably be a better name). As a result it is terribly slow on very large training sets (but we will see much faster Gradient Descent algorithms shortly). However, Gradient Descent scales well with the number of features; training a Linear Regression model when there are hundreds of thousands of features is much faster using Gradient Descent than using the Normal Equation or SVD decomposition.

Once you have the gradient vector, which points uphill, just go in the opposite direction to go downhill. This means subtracting $\nabla_{\boldsymbol{\theta}}\text{MSE}(\boldsymbol{\theta})$ from $\boldsymbol{\theta}$. This is where the learning rate η comes into play:[3] multiply the gradient vector by η to determine the size of the downhill step (Equation 4-7).

Equation 4-7. Gradient Descent step

$$\boldsymbol{\theta}^{(\text{next step})} = \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} \text{MSE}\left(\boldsymbol{\theta}\right)$$

Let's look at a quick implementation of this algorithm:

```
eta = 0.1  # learning rate
n_epochs = 1000
m = len(X_b)  # number of instances

np.random.seed(42)
theta = np.random.randn(2, 1)  # randomly initialized model parameters

for epoch in range(n_epochs):
```

```
    gradients = 2 / m * X_b.T @ (X_b @ theta - y)
    theta = theta - eta * gradients
```

That wasn't too hard! Each iteration over the training set is called an *epoch*. Let's look at the resulting `theta`:

```
>>> theta
array([[4.21509616],
       [2.77011339]])
```

Hey, that's exactly what the Normal Equation found! Gradient Descent worked perfectly. But what if you had used a different learning rate `eta`? Figure 4-8 shows the first 20 steps of Gradient Descent using three different learning rates. The line at the bottom of each plot represents the random starting point, then each epoch is represented by a darker and darker line.

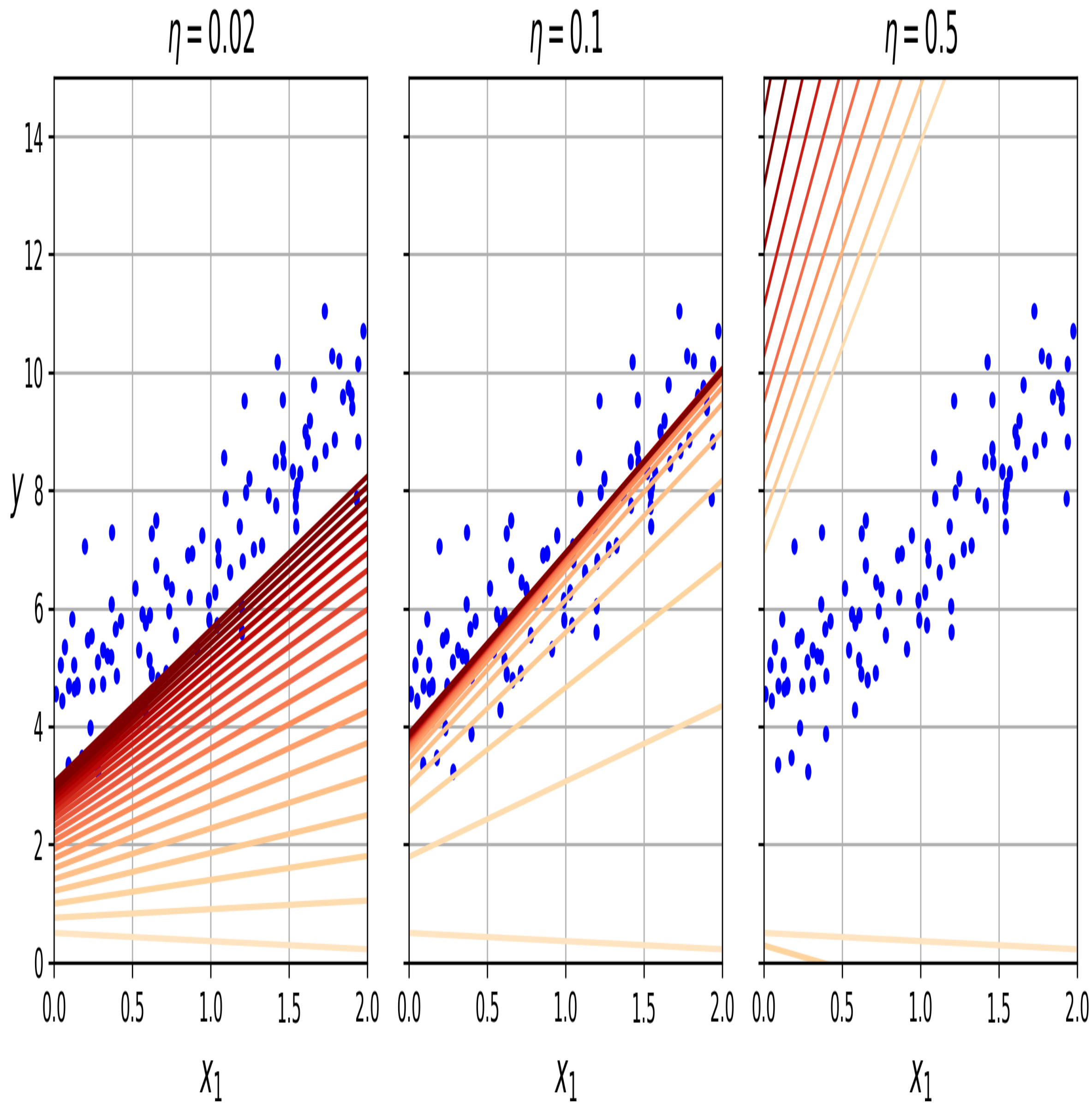


Figure 4-8. Gradient Descent with various learning rates

On the left, the learning rate is too low: the algorithm will eventually reach the solution, but it will take a long time. In the middle, the learning rate looks pretty good: in just a few epochs, it has already converged to the solution. On the right, the learning rate is too high: the algorithm diverges, jumping all over the place and actually getting further and further away from the solution at every step.

To find a good learning rate, you can use grid search (see Chapter 2). However, you may want to limit the number of epochs so that grid search can eliminate models that take too long to converge.

You may wonder how to set the number of epochs. If it is too low, you will still be far away from the optimal solution when the algorithm stops; but if it is too high, you will waste time while the model parameters do not change anymore. A simple solution is to set a very large number of epochs but to interrupt the algorithm when the gradient vector becomes tiny—that is, when its norm becomes smaller than a tiny number ϵ (called the *tolerance*)—because this happens when Gradient Descent has (almost) reached the minimum.

CONVERGENCE RATE

When the cost function is convex and its slope does not change abruptly (as is the case for the MSE cost function), Batch Gradient Descent with a fixed learning rate will eventually converge to the optimal solution, but you may have to wait a while: it can take $O(1/\epsilon)$ iterations to reach the optimum within a range of ϵ, depending on the shape of the cost function. If you divide the tolerance by 10 to have a more precise solution, then the algorithm may have to run about 10 times longer.

Stochastic Gradient Descent

The main problem with Batch Gradient Descent is the fact that it uses the whole training set to compute the gradients at every step, which makes it very slow when the training set is large. At the opposite extreme, *Stochastic Gradient Descent* picks a random instance in the training set at every step and computes the gradients based only on that single instance. Obviously, working on a single instance at a time makes the algorithm much faster because it has very little data to manipulate at every iteration. It also makes it possible to train on huge training sets, since only one instance needs to be in memory at each iteration (Stochastic GD can be implemented as an out-of-core algorithm; see Chapter 1).

On the other hand, due to its stochastic (i.e., random) nature, this algorithm is much less regular than Batch Gradient Descent: instead of gently decreasing until it reaches the minimum, the cost function will bounce up and down, decreasing only on average. Over time it will end up very close to the minimum, but once it gets there it will continue to bounce around, never settling down (see Figure 4-9). So once the algorithm stops, the final parameter values are good, but not optimal.

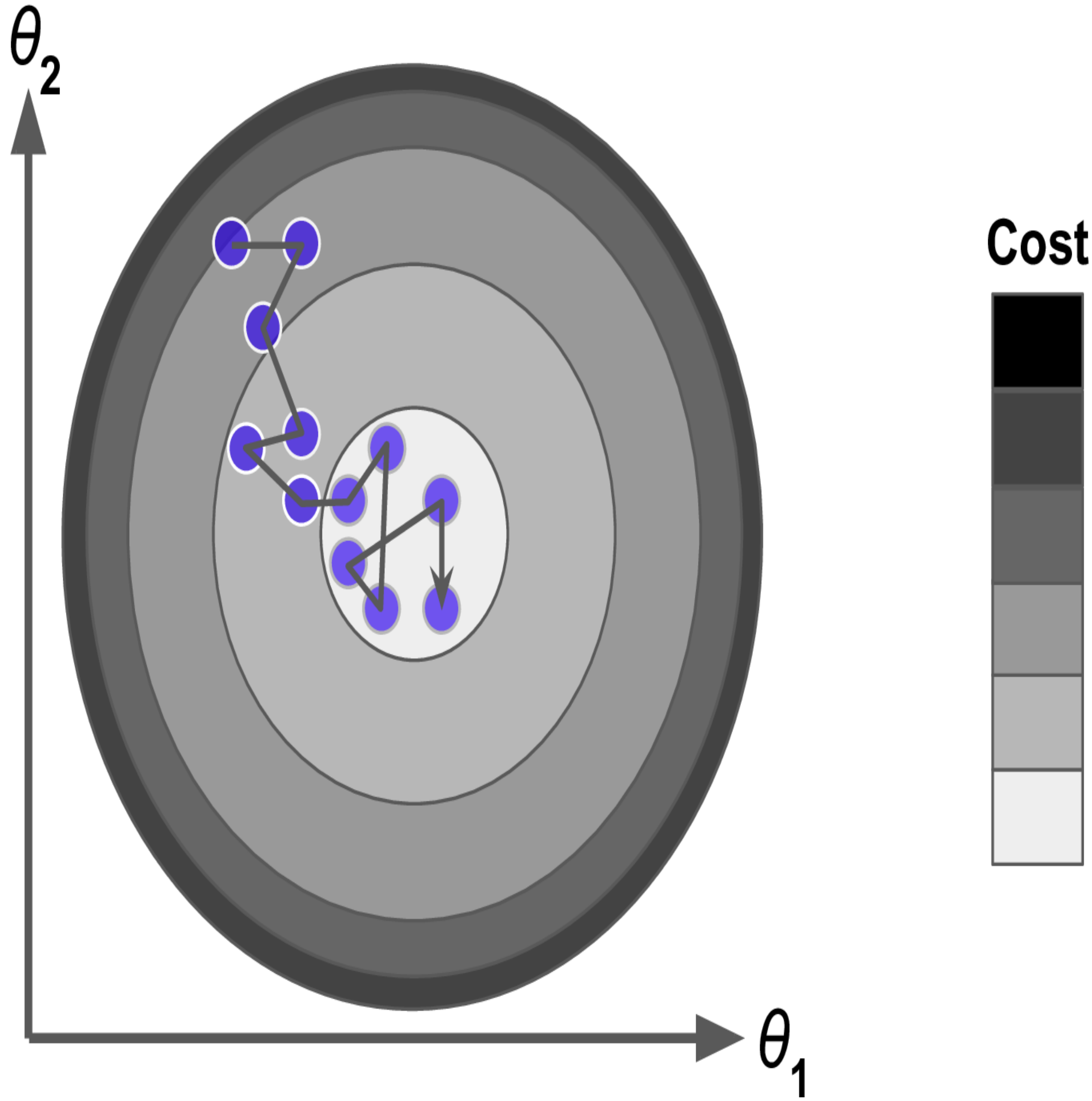


Figure 4-9. With Stochastic Gradient Descent, each training step is much faster but also much more stochastic than when using Batch Gradient Descent

When the cost function is very irregular (as in Figure 4-6), this can actually help the algorithm jump out of local minima, so Stochastic Gradient Descent has a better chance of finding the global minimum than Batch Gradient Descent does.

Therefore, randomness is good to escape from local optima, but bad because it means that the algorithm can never settle at the minimum. One solution to this dilemma is to gradually reduce the learning rate. The steps start out large (which helps make quick progress and escape local minima), then get smaller and smaller, allowing the algorithm to settle at the global minimum. This process is akin to *simulated annealing*, an algorithm inspired from the process in metallurgy of annealing, where molten metal is slowly cooled down. The function that determines the learning rate at each iteration is called the *learning schedule*. If the learning rate is reduced too quickly, you may get stuck in a local minimum, or even end up frozen halfway to the minimum. If the learning rate is reduced too slowly, you may jump around the minimum for a long time and end up with a suboptimal solution if you halt training too early.

This code implements Stochastic Gradient Descent using a simple learning schedule:

```
n_epochs = 50
t0, t1 = 5, 50  # learning schedule hyperparameters

def learning_schedule(t):
    return t0 / (t + t1)

np.random.seed(42)
theta = np.random.randn(2, 1)  # random initialization

for epoch in range(n_epochs):
    for iteration in range(m):
        random_index = np.random.randint(m)
        xi = X_b[random_index : random_index + 1]
        yi = y[random_index : random_index + 1]
        gradients = 2 * xi.T @ (xi @ theta - yi)  # for SGD, do not divide by m
        eta = learning_schedule(epoch * m + iteration)
        theta = theta - eta * gradients
```

By convention we iterate by rounds of *m* iterations; each round is called an *epoch*, as earlier. While the Batch Gradient Descent code iterated 1,000 times through the whole training set, this code goes through the training set only 50 times and reaches a pretty good solution:

```
>>> theta
array([[4.21076011],
       [2.74856079]])
```

Figure 4-10 shows the first 20 steps of training (notice how irregular the steps are).

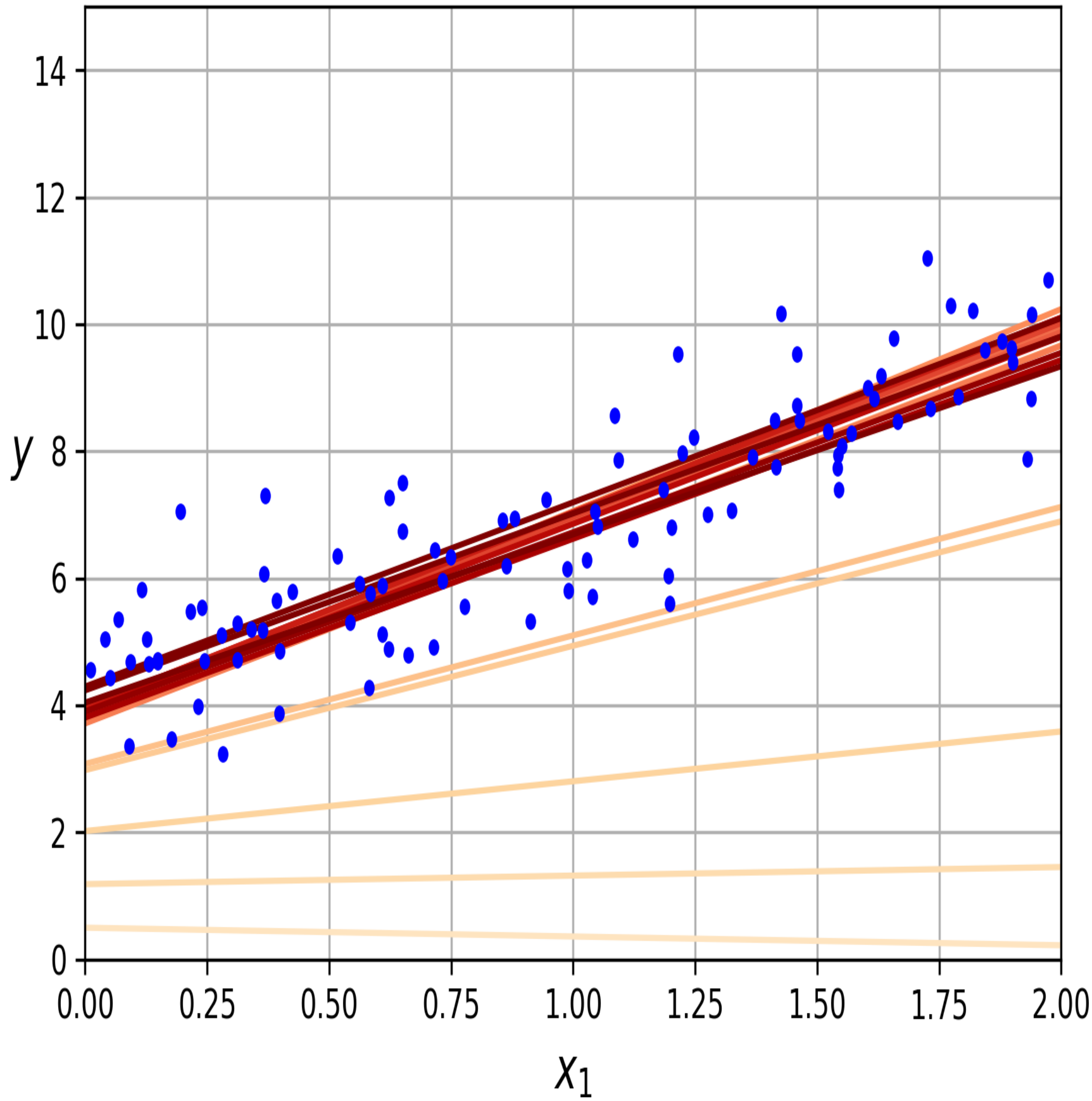


Figure 4-10. The first 20 steps of Stochastic Gradient Descent

Note that since instances are picked randomly, some instances may be picked several times per epoch, while others may not be picked at all. If you want to be sure that the algorithm goes through every instance at each epoch, another approach is to shuffle the training set (making sure to shuffle the input features and the labels jointly), then go through it instance by instance, then shuffle it again, and so on. However, this approach is more complex and it generally does not improve the result.

WARNING

When using Stochastic Gradient Descent, the training instances must be independent and identically distributed (IID) to ensure that the parameters get pulled toward the global optimum, on average. A simple way to ensure this is to shuffle the instances during training (e.g., pick each instance randomly, or shuffle the training set at the beginning of each epoch). If you do not shuffle the instances—for example, if the instances are sorted by label—then SGD will start by optimizing for one label, then the next, and so on, and it will not settle close to the global minimum.

To perform Linear Regression using Stochastic GD with Scikit-Learn, you can use the `SGDRegressor` class, which defaults to optimizing the MSE cost function. The following code runs for maximum 1,000 epochs (`max_iter`) or until the loss drops by less than 10^{-5} (`tol`) during 100 epochs (`n_iter_no_change`). It starts with a learning rate of 0.01 (`eta0`), using the default learning schedule (different from the one we used). Lastly, it does not use any regularization (`penalty=None`; more details on this shortly):

```
from sklearn.linear_model import SGDRegressor

sgd_reg = SGDRegressor(max_iter=1000, tol=1e-5, penalty=None, eta0=0.01,
                       n_iter_no_change=100, random_state=42)
sgd_reg.fit(X, y.ravel())  # y.ravel() because fit() expects 1D targets
```

Once again, you find a solution quite close to the one returned by the Normal Equation:

```
>>> sgd_reg.intercept_, sgd_reg.coef_
(array([4.21278812]), array([2.77270267]))
```

TIP

All Scikit-Learn estimators can be trained using the `fit()` method, but some estimators also have a `partial_fit()` method that you can call to run a single round of training on one or more instances (it ignores hyperparameters like `max_iter` or `tol`). Repeatedly calling `partial_fit()` will gradually train the model. This is useful when you need more control over the training process. Other models have a `warm_start` hyperparameter instead (and some have both): if you set `warm_start=True`, calling the `fit()` method on a trained model will not reset the model, it will just continue training where it left off, respecting hyperparameters like `max_iter` and `tol`. Note that `fit()` resets the iteration counter used by the learning schedule, while `partial_fit()` does not.

Mini-batch Gradient Descent

The last Gradient Descent algorithm we will look at is called *Mini-batch Gradient Descent*. It is straightforward once you know Batch and Stochastic Gradient Descent: at each step, instead of computing the gradients based on the full training set (as in Batch GD) or based on just one instance (as in Stochastic GD), Mini-batch GD computes the gradients on small random sets of instances called *mini-batches*. The main advantage of Mini-batch GD over Stochastic GD is that you can get a performance boost from hardware optimization of matrix operations, especially when using GPUs.

The algorithm's progress in parameter space is less erratic than with Stochastic GD, especially with fairly large mini-batches. As a result, Mini-batch GD will end up walking around a bit closer to the minimum than Stochastic GD—but it may be harder for it to escape from local minima (in the case of problems that suffer from local minima, unlike Linear Regression with the MSE cost function). Figure 4-11 shows the paths taken by the three Gradient Descent algorithms in parameter space during training. They all end up near the minimum, but Batch GD's path actually stops at the minimum, while both Stochastic GD and Mini-batch GD continue to walk around. However, don't forget that Batch GD takes a lot of time to take each step, and Stochastic GD and Mini-batch GD would also reach the minimum if you used a good learning schedule.

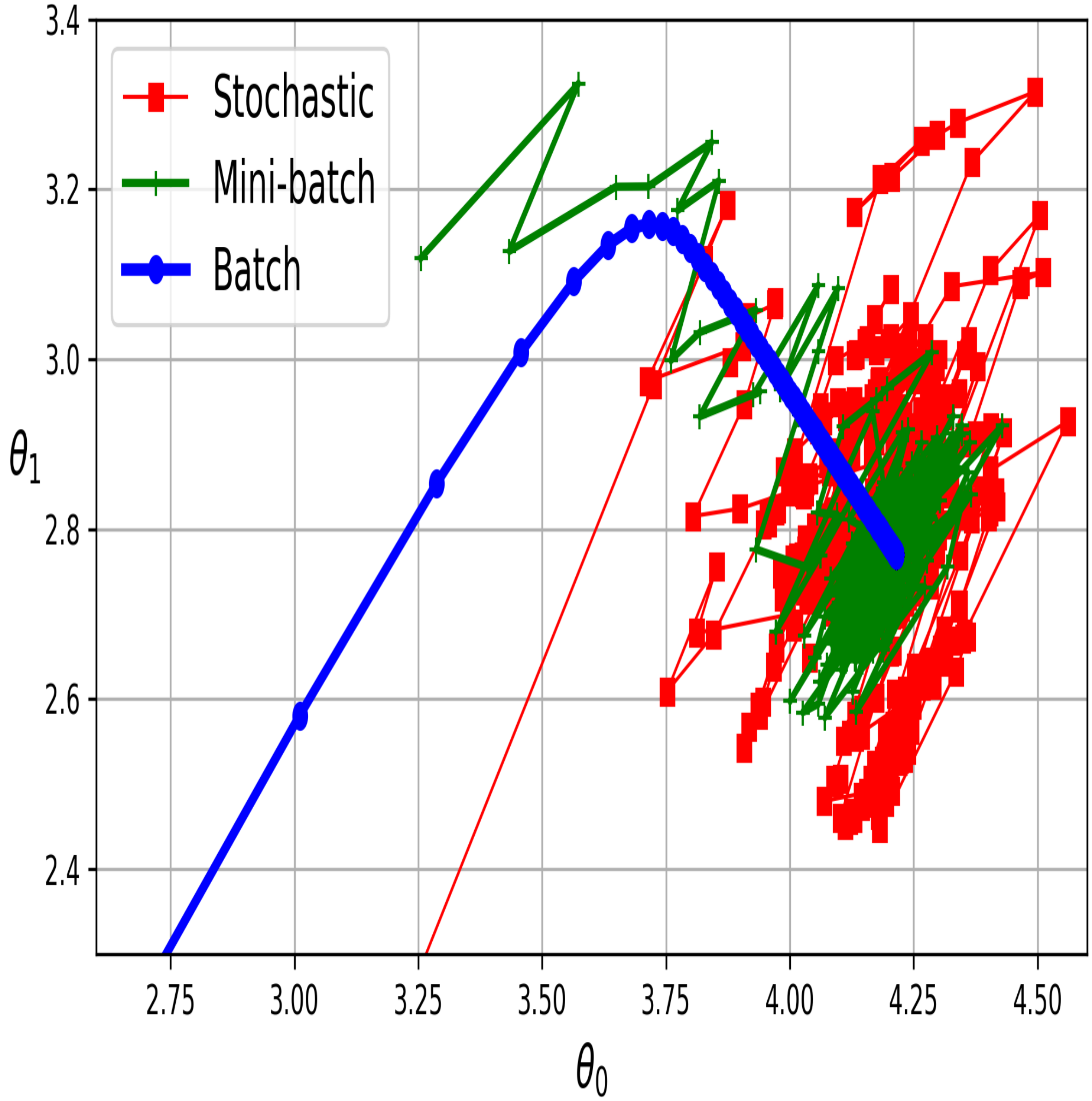


Figure 4-11. Gradient Descent paths in parameter space

Let's compare the algorithms we've discussed so far for Linear Regression[4] (recall that *m* is the number of training instances and *n* is the number of features); see Table 4-1.

Table 4-1. Comparison of algorithms for Linear Regres

s
i
o
n

Algorithm	Large *m*	Out-of-core support	Large *n*	Hyperparams	Scaling required	Scikit-Learn
Normal Equation	Fast	No	Slow	0	No	N/A
SVD	Fast	No	Slow	0	No	`LinearRegression`
Batch GD	Slow	No	Fast	2	Yes	N/A
Stochastic GD	Fast	Yes	Fast	≥2	Yes	`SGDRegressor`
Mini-batch GD	Fast	Yes	Fast	≥2	Yes	N/A

There is almost no difference after training: all these algorithms end up with very similar models and make predictions in exactly the same way.

Polynomial Regression

What if your data is more complex than a straight line? Surprisingly, you can use a linear model to fit nonlinear data. A simple way to do this is to add powers of each feature as new features, then train a linear model on this extended set of features. This technique is called *Polynomial Regression*.

Let's look at an example. First, let's generate some nonlinear data, based on a simple *quadratic equation*[5] (plus some noise; see Figure 4-12):

```
np.random.seed(42)
m = 100
X = 6 * np.random.rand(m, 1) - 3
y = 0.5 * X ** 2 + X + 2 + np.random.randn(m, 1)
```

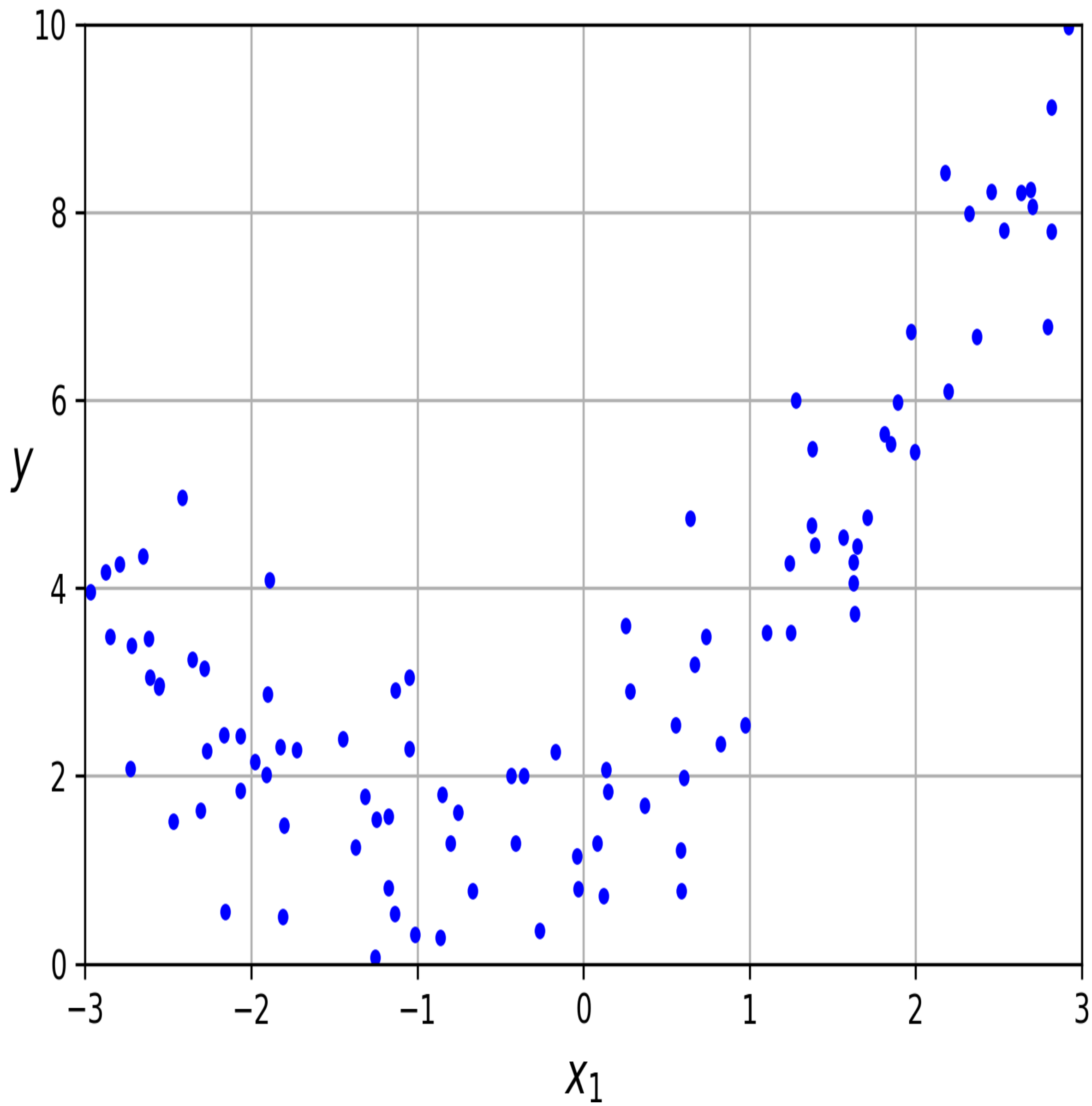


Figure 4-12. Generated nonlinear and noisy dataset

Clearly, a straight line will never fit this data properly. So let's use Scikit-Learn's `PolynomialFeatures` class to transform our training data, adding the square (second-degree polynomial) of each feature in the training set as a new feature (in this case there is just one feature):

```
>>> from sklearn.preprocessing import PolynomialFeatures
>>> poly_features = PolynomialFeatures(degree=2, include_bias=False)
>>> X_poly = poly_features.fit_transform(X)
>>> X[0]
array([-0.75275929])
>>> X_poly[0]
array([-0.75275929,  0.56664654])
```

`X_poly` now contains the original feature of `X` plus the square of this feature. Now you can fit a `LinearRegression` model to this extended training data (Figure 4-13):

```
>>> lin_reg = LinearRegression()
>>> lin_reg.fit(X_poly, y)
>>> lin_reg.intercept_, lin_reg.coef_
(array([1.78134581]), array([[0.93366893, 0.56456263]]))
```

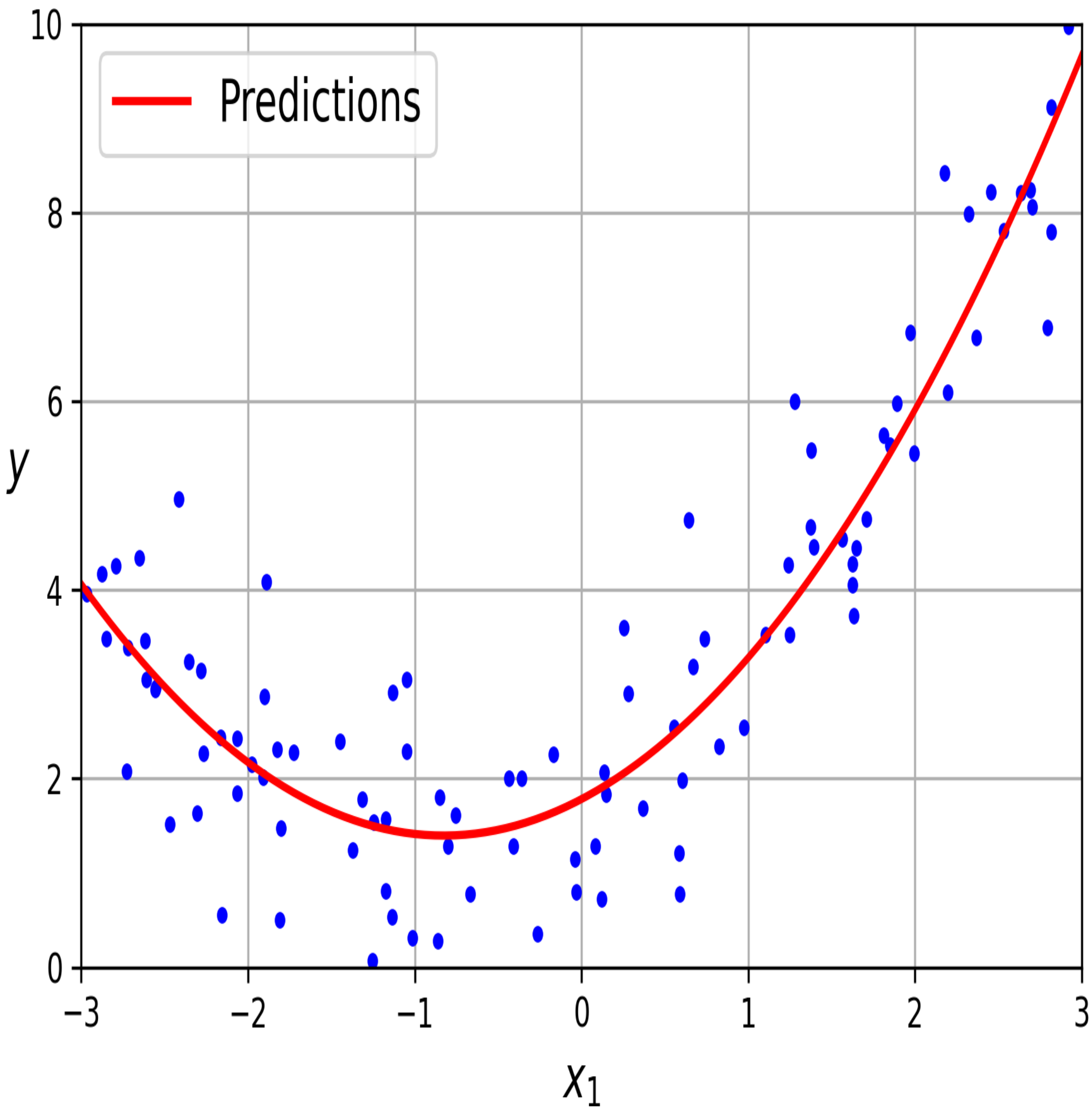


Figure 4-13. Polynomial Regression model predictions

Not bad: the model estimates $\hat{y} = 0.56{x_1}^2 + 0.93x_1 + 1.78$ when in fact the original function was $y = 0.5{x_1}^2 + 1.0x_1 + 2.0 + \text{Gaussian noise}$.

Note that when there are multiple features, Polynomial Regression is capable of finding relationships between features, which is something a plain Linear Regression model cannot do. This is made possible by the fact that `PolynomialFeatures` also adds all combinations of features up to the given degree. For example, if there were two features a and b, `PolynomialFeatures` with `degree=3` would not only add the features a^2, a^3, b^2, and b^3, but also the combinations ab, a^2b, and ab^2.

> **WARNING**
>
> `PolynomialFeatures(degree=d)` transforms an array containing n features into an array containing $(n + d)! / d!n!$ features, where $n!$ is the *factorial* of n, equal to $1 \times 2 \times 3 \times \cdots \times n$. Beware of the combinatorial explosion of the number of features!

Learning Curves

If you perform high-degree Polynomial Regression, you will likely fit the training data much better than with plain Linear Regression. For example, Figure 4-14 applies a 300-degree polynomial model to the preceding training data, and compares the result with a pure linear model and a quadratic model (second-degree polynomial). Notice how the 300-degree polynomial model wiggles around to get as close as possible to the training instances.

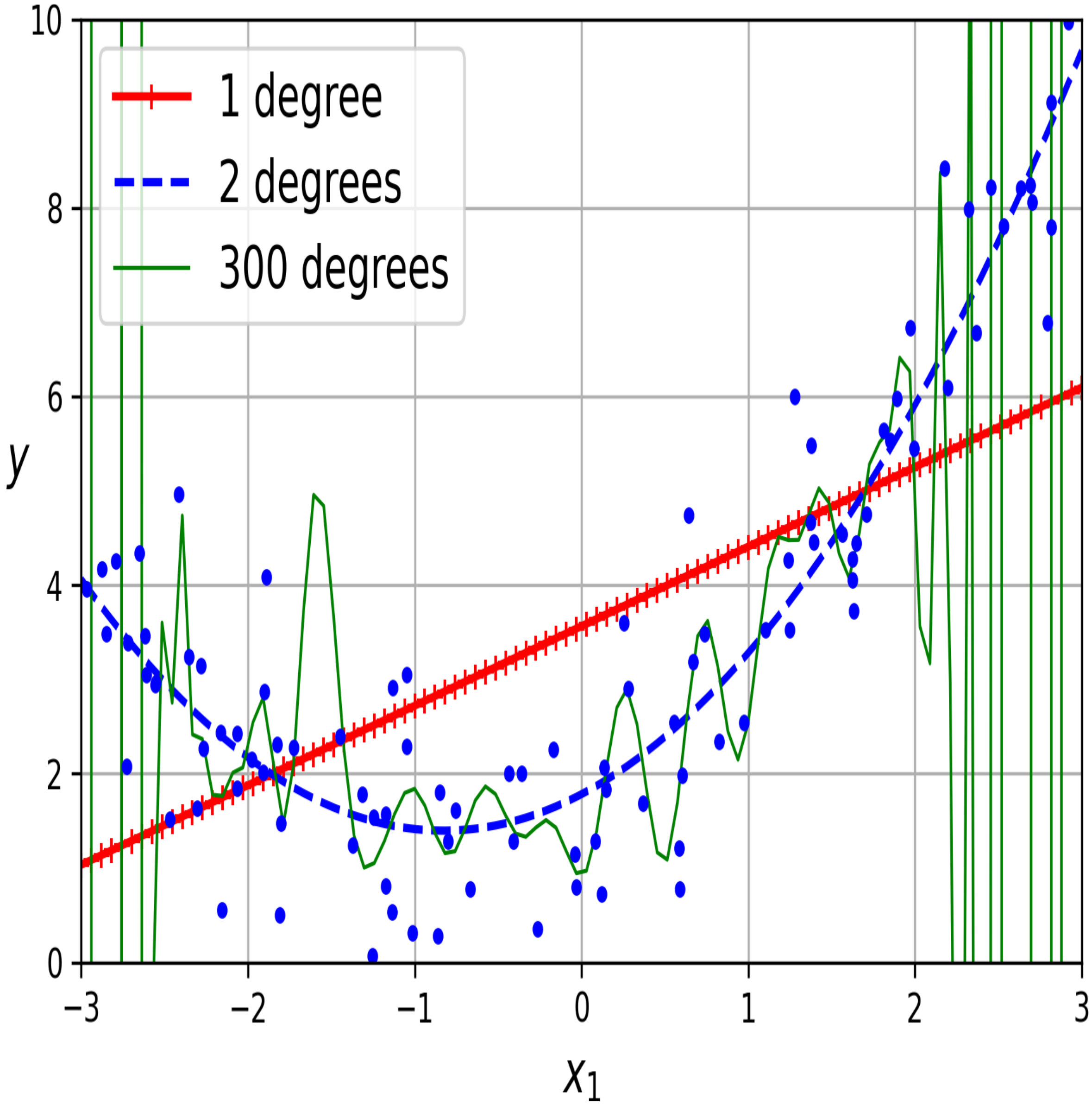


Figure 4-14. High-degree Polynomial Regression

This high-degree Polynomial Regression model is severely overfitting the training data, while the linear model is underfitting it. The model that will generalize best in this case is the quadratic model, which makes sense because the data was generated using a quadratic model. But in general you won't know what function generated the data, so how can you decide how complex your model should be? How can you tell that your model is overfitting or underfitting the data?

In Chapter 2 you used cross-validation to get an estimate of a model's generalization performance. If a model performs well on the training data but generalizes poorly according to the cross-validation metrics, then your model is overfitting. If it performs poorly on both, then it is underfitting. This is one way to tell when a model is too simple or too complex.

Another way to tell is to look at the *learning curves*: these are plots of the model's training error and validation error as a function of the training iteration: just evaluate the model at regular intervals during training on both the training set and the validation set, and plot the results. If the model cannot be trained incrementally (i.e., if it does not support `partial_fit()` or `warm_start`), then you must train the model several times on gradually larger subsets of the training set.

Scikit-Learn has a useful `learning_curve()` function to help with this: it trains and evaluates the model using cross-validation. By default it retrains the model on growing subsets of the training set, but if the model supports incremental learning you can set `exploit_incremental_learning=True` when calling `learning_curve()` and it will train the model incrementally instead. The function returns the training set sizes at which it evaluated the model, and the training and validation scores it measured for each size and for each cross-validation fold. Let's use this function to look at the learning curves of the plain Linear Regression model (see Figure 4-15):

```
from sklearn.model_selection import learning_curve

train_sizes, train_scores, valid_scores = learning_curve(
    LinearRegression(), X, y, train_sizes=np.linspace(0.01, 1.0, 40), cv=5,
    scoring="neg_root_mean_squared_error")
train_errors = -train_scores.mean(axis=1)
valid_errors = -valid_scores.mean(axis=1)

plt.plot(train_sizes, train_errors, "r-+", linewidth=2, label="train")
plt.plot(train_sizes, valid_errors, "b-", linewidth=3, label="valid")
[...]  # beautify the figure: add labels, axis, grid and legend.
plt.show()
```

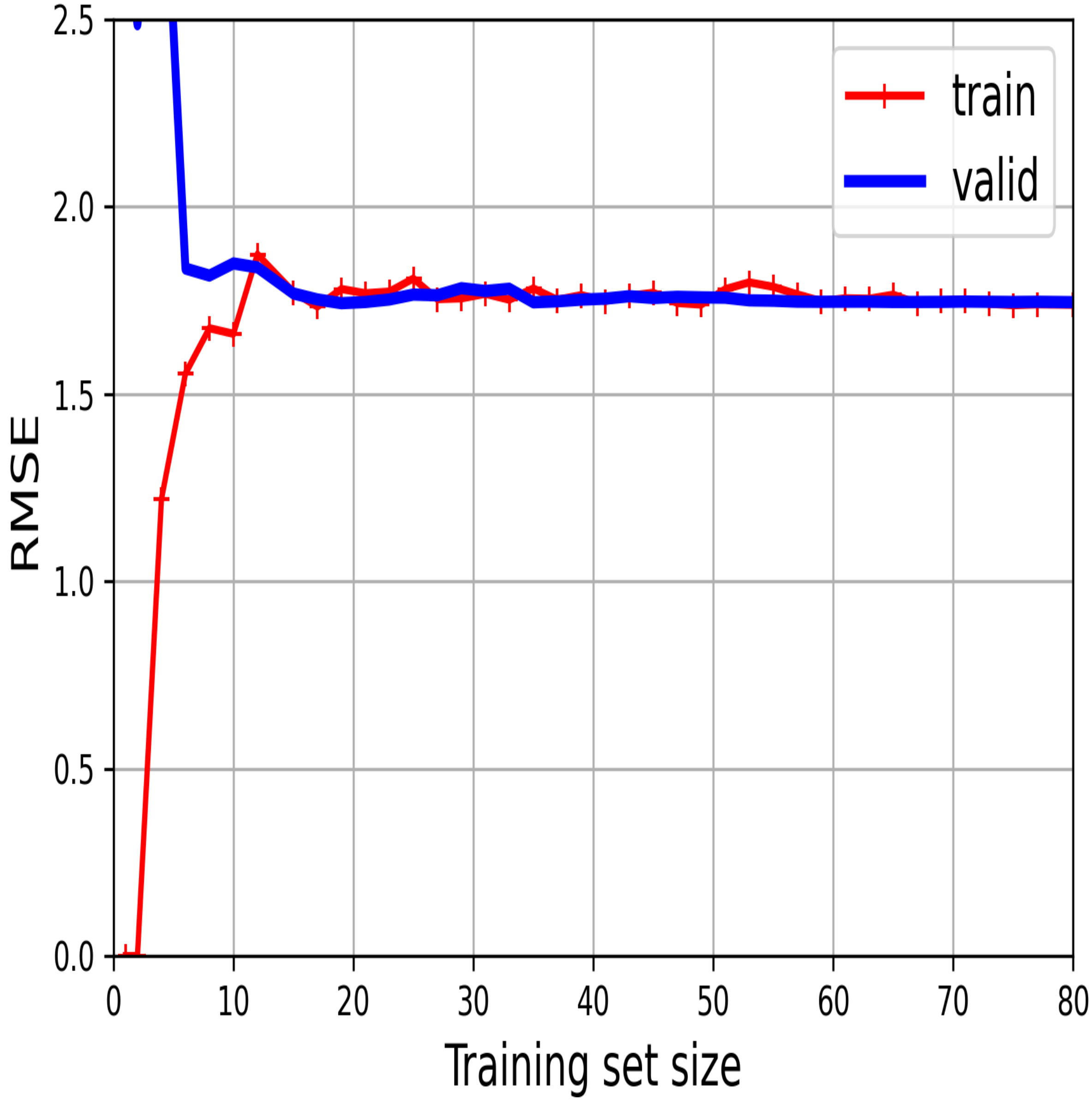


Figure 4-15. Learning curves

This model is underfitting, let's see why. First, let's look at the training error: when there are just one or two instances in the training set, the model can fit them perfectly, which is why the curve starts at zero. But as new instances are added to the training set, it becomes impossible for the model to fit the training data perfectly, both because the data is noisy and because it is not linear at all. So the error on the training data goes up until it reaches a plateau, at which point adding new instances to the training set doesn't make the average error much better or worse. Now let's look at the validation error. When the model is trained on very few training instances, it is incapable of generalizing properly, which is why the validation error is initially quite large. Then, as the model is shown more training examples, it learns, and thus the validation error slowly goes down. However, once again a straight line cannot do a good job modeling the data, so the error ends up at a plateau, very close to the other curve.

These learning curves are typical of a model that's underfitting. Both curves have reached a plateau; they are close and fairly high.

TIP

If your model is underfitting the training data, adding more training examples will not help. You need to use a better model or come up with better features.

Now let's look at the learning curves of a 10th-degree polynomial model on the same data (Figure 4-16):

```
from sklearn.pipeline import make_pipeline

polynomial_regression = make_pipeline(
    PolynomialFeatures(degree=10, include_bias=False),
    LinearRegression())

train_sizes, train_scores, valid_scores = learning_curve(
    polynomial_regression, X, y, train_sizes=np.linspace(0.01, 1.0, 40), cv=5,
    scoring="neg_root_mean_squared_error")
[...]  # same as earlier
```

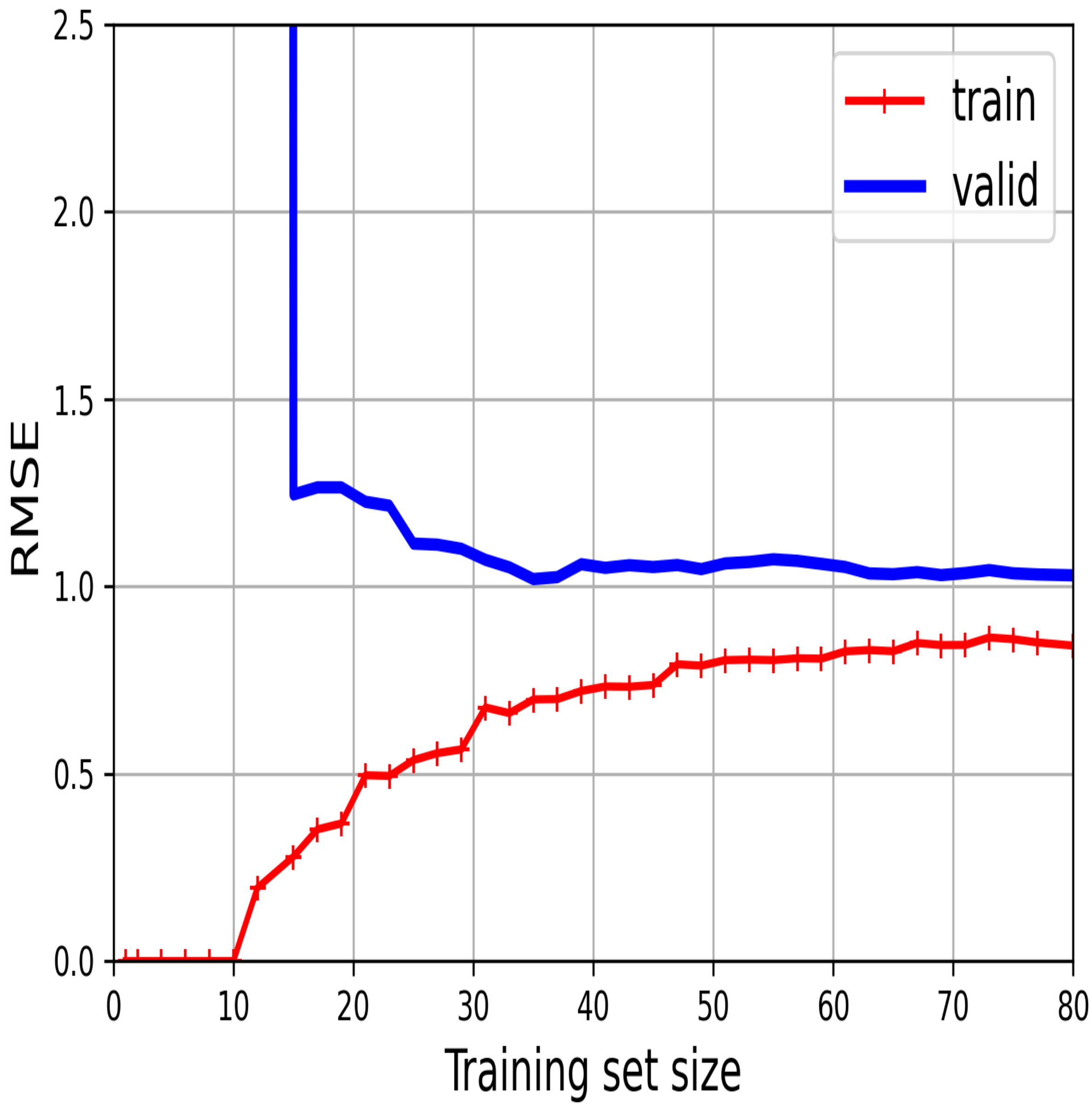


Figure 4-16. Learning curves for the 10th-degree polynomial model

These learning curves look a bit like the previous ones, but there are two very important differences:

- The error on the training data is much lower than before.
- There is a gap between the curves. This means that the model performs significantly better on the training data than on the validation data, which is the hallmark of an overfitting model. If you used a much larger training set, however, the two curves would continue to get closer.

TIP

One way to improve an overfitting model is to feed it more training data until the validation error reaches the training error.

THE BIAS/VARIANCE TRADE-OFF

An important theoretical result of statistics and Machine Learning is the fact that a model's generalization error can be expressed as the sum of three very different errors:

Bias

This part of the generalization error is due to wrong assumptions, such as assuming that the data is linear when it is actually quadratic. A high-bias model is most likely to underfit the training data.[6]

Variance

This part is due to the model's excessive sensitivity to small variations in the training data. A model with many degrees of freedom (such as a high-degree polynomial model) is likely to have high variance and thus overfit the training data.

Irreducible error

This part is due to the noisiness of the data itself. The only way to reduce this part of the error is to clean up the data (e.g., fix the data sources, such as broken sensors, or detect and remove outliers).

Increasing a model's complexity will typically increase its variance and reduce its bias. Conversely, reducing a model's complexity increases its bias and reduces its variance. This is why it is called a trade-off.

Regularized Linear Models

As we saw in Chapters 1 and 2, a good way to reduce overfitting is to regularize the model (i.e., to constrain it): the fewer degrees of freedom it has, the harder it will be for it to overfit the data. A simple way to regularize a polynomial model is to reduce the number of polynomial degrees.

For a linear model, regularization is typically achieved by constraining the weights of the model. We will now look at Ridge Regression, Lasso Regression, and Elastic Net, which implement three different ways to constrain the weights.

Ridge Regression

Ridge Regression (also called *Tikhonov regularization*) is a regularized version of Linear Regression: a *regularization term* equal to $\frac{\alpha}{m}\sum_{i=1}^{n}{\theta_i}^2$ is added to the MSE. This forces the learning algorithm to not only fit the data but also keep the model weights as small as possible. Note that the regularization term should only be added to the cost function during training. Once the model is trained, you want to use the unregularized MSE (or the RMSE) to evaluate the model's performance.

The hyperparameter α controls how much you want to regularize the model. If $\alpha = 0$, then Ridge Regression is just Linear Regression. If α is very large, then all weights end up very close to zero and the result is a flat line going through the data's mean. Equation 4-8 presents the Ridge Regression cost function.[7]

Equation 4-8. Ridge Regression cost function

$$J(\boldsymbol{\theta}) = \text{MSE}(\boldsymbol{\theta}) + \frac{\alpha}{m}\sum_{i=1}^{n}{\theta_i}^2$$

Note that the bias term θ_0 is not regularized (the sum starts at $i = 1$, not 0). If we define $\mathbf{w}$ as the vector of feature weights (θ_1 to θ_n), then the regularization term is equal to $\alpha(\| \mathbf{w} \|_2)^2 / m$, where $\| \mathbf{w} \|_2$ represents the ℓ_2 norm of the weight vector.[8] For Batch Gradient Descent, just add $2\alpha\mathbf{w} / m$ to the part of the MSE gradient vector that corresponds to the feature weights, without adding anything to the gradient of the bias term (see Equation 4-6).

> **WARNING**
>
> It is important to scale the data (e.g., using a `StandardScaler`) before performing Ridge Regression, as it is sensitive to the scale of the input features. This is true of most regularized models.

Figure 4-17 shows several Ridge models trained on some very noisy linear data using different α values. On the left, plain Ridge models are used, leading to linear predictions. On the right, the data is first expanded using `PolynomialFeatures(degree=10)`, then it is scaled using a `StandardScaler`, and finally the Ridge models are applied to the resulting features: this is Polynomial Regression with Ridge regularization. Note how increasing α leads to flatter (i.e., less extreme, more reasonable) predictions, thus reducing the model's variance but increasing its bias.

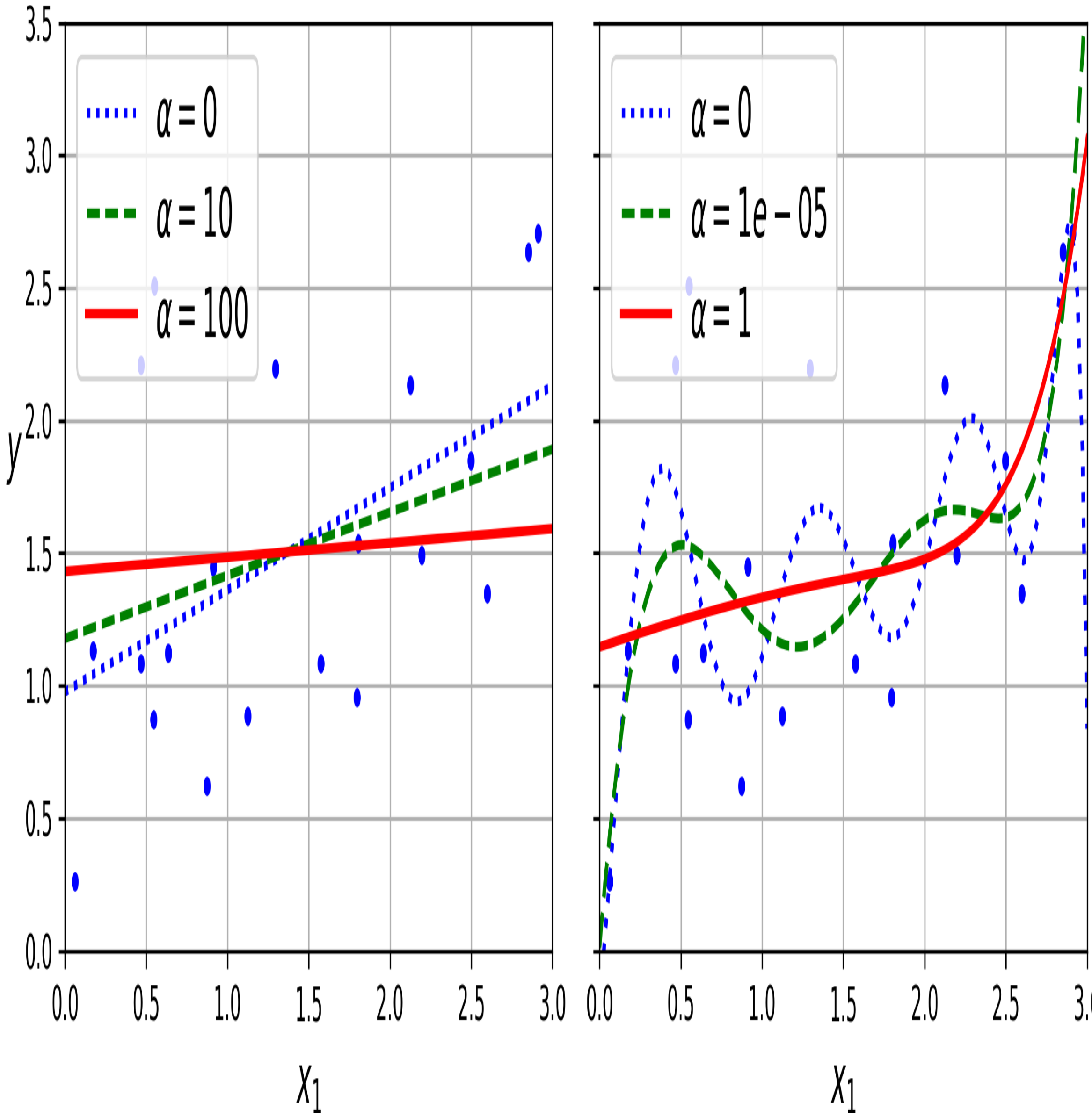


Figure 4-17. A linear model (left) and a polynomial model (right), both with various levels of Ridge regularization

As with Linear Regression, we can perform Ridge Regression either by computing a closed-form equation or by performing Gradient Descent. The pros and cons are the same. Equation 4-9 shows the closed-form solution, where **A** is the $(n + 1) \times (n + 1)$ *identity matrix*,[9] except with a 0 in the top-left cell, corresponding to the bias term.

Equation 4-9. Ridge Regression closed-form solution

$$\widehat{\boldsymbol{\theta}} = \left(\mathbf{X}^\intercal \mathbf{X} + \alpha \mathbf{A}\right)^{-1} \mathbf{X}^\intercal \ \mathbf{y}$$

Here is how to perform Ridge Regression with Scikit-Learn using a closed-form solution (a variant of Equation 4-9 that uses a matrix factorization technique by André-Louis Cholesky):

```
>>> from sklearn.linear_model import Ridge
>>> ridge_reg = Ridge(alpha=0.1, solver="cholesky")
>>> ridge_reg.fit(X, y)
```

```
>>> ridge_reg.predict([[1.5]])
array([[1.55325833]])
```

And using Stochastic Gradient Descent:[10]

```
>>> sgd_reg = SGDRegressor(penalty="l2", alpha=0.1 / m, tol=None,
...                        max_iter=1000, eta0=0.01, random_state=42)
...
>>> sgd_reg.fit(X, y.ravel())  # y.ravel() because fit() expects 1D targets
>>> sgd_reg.predict([[1.5]])
array([1.55302613])
```

The `penalty` hyperparameter sets the type of regularization term to use. Specifying `"l2"` indicates that you want SGD to add a regularization term to the MSE cost function equal to `alpha` times the square of the ℓ_2 norm of the weight vector: this is just like Ridge Regression, except there's no division by *m* in this case, which is why we passed `alpha=0.1 / m`, to get the same result as `Ridge(alpha=0.1)`.

> **TIP**
>
> The `RidgeCV` class also performs Ridge Regression, but it automatically tunes hyperparameters using cross-validation. It's roughly equivalent to using `GridSearchCV`, but it's optimized for Ridge Regression and runs *much* faster. Several other estimators (mostly linear) also have efficient CV variants, such as `LassoCV` or `ElasticNetCV`.

Lasso Regression

Least Absolute Shrinkage and Selection Operator Regression (usually simply called *Lasso Regression*) is another regularized version of Linear Regression: just like Ridge Regression, it adds a regularization term to the cost function, but it uses the ℓ_1 norm of the weight vector instead of the square of the ℓ_2 norm (see Equation 4-10). Notice that the ℓ_1 norm is multiplied by 2_α*, whereas the* ℓ_2 *norm was multiplied by* _α / *m* in Ridge regression. These factors were chosen to ensure that the optimal α value is independent from the training set size: different norms lead to different factors (see Scikit-Learn issue #15657 for more details).

Equation 4-10. Lasso Regression cost function

$$J(\boldsymbol{\theta}) = \mathrm{MSE}(\boldsymbol{\theta}) + 2\alpha \sum_{i=1}^{n} |\theta_i|$$

Figure 4-18 shows the same thing as Figure 4-17 but replaces Ridge models with Lasso models and uses different α values.

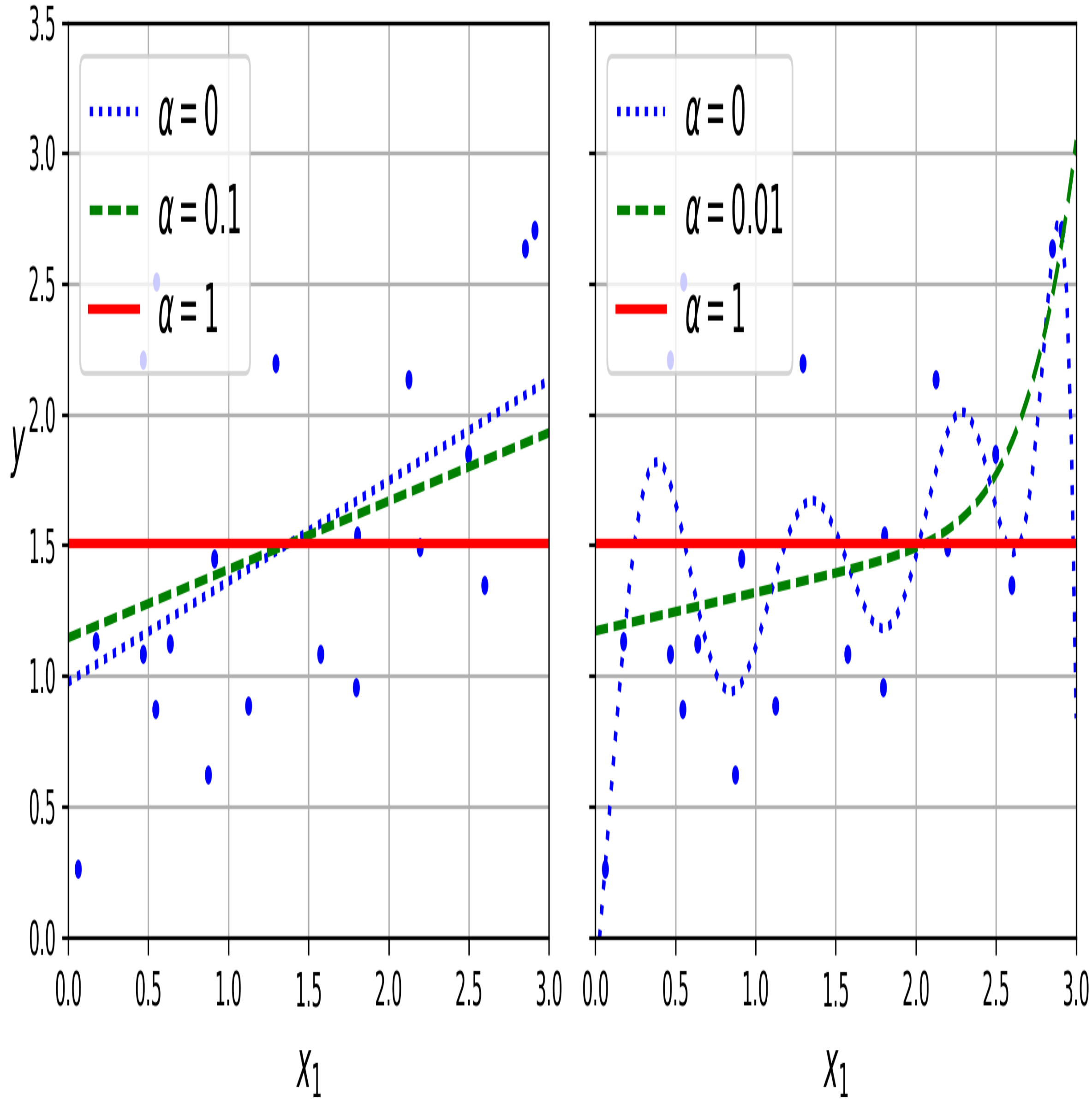


Figure 4-18. A linear model (left) and a polynomial model (right), both using various levels of Lasso regularization

An important characteristic of Lasso Regression is that it tends to eliminate the weights of the least important features (i.e., set them to zero). For example, the dashed line in the righthand plot in Figure 4-18 (with $\alpha = 0.01$) looks roughly cubic: all the weights for the high-degree polynomial features are equal to zero. In other words, Lasso Regression automatically performs feature selection and outputs a *sparse model* (i.e., with few nonzero feature weights).

You can get a sense of why this is the case by looking at Figure 4-19: the axes represent two model parameters, and the background contours represent different loss functions. In the top-left plot, the contours represent the ℓ_1 loss ($|\theta_1| + |\theta_2|$), which drops linearly as you get closer to any axis. For example, if you initialize the model parameters to $\theta_1 = 2$ and $\theta_2 = 0.5$, running Gradient Descent will decrement both parameters equally (as represented by the dashed yellow line); therefore θ_2 will reach 0 first (since it was closer to 0 to begin with). After that, Gradient Descent will roll down the gutter until it reaches $\theta_1 = 0$ (with a bit of bouncing around, since the gradients of ℓ_1 never get close to 0: they are either –1 or 1 for each parameter). In the top-right plot, the contours represent Lasso's cost function (i.e., an MSE cost function plus an ℓ_1 loss). The small white circles show the path that Gradient Descent takes to optimize some model parameters that were initialized around $\theta_1 = 0.25$ and $\theta_2 = -1$: notice once again how the path quickly reaches $\theta_2 = 0$, then rolls down the gutter and ends up bouncing around the global optimum (represented by the red square). If we increased α, the global optimum would move left along the dashed yellow line, while if we decreased α, the global optimum would move right (in this example, the optimal parameters for the unregularized MSE are $\theta_1 = 2$ and $\theta_2 = 0.5$).

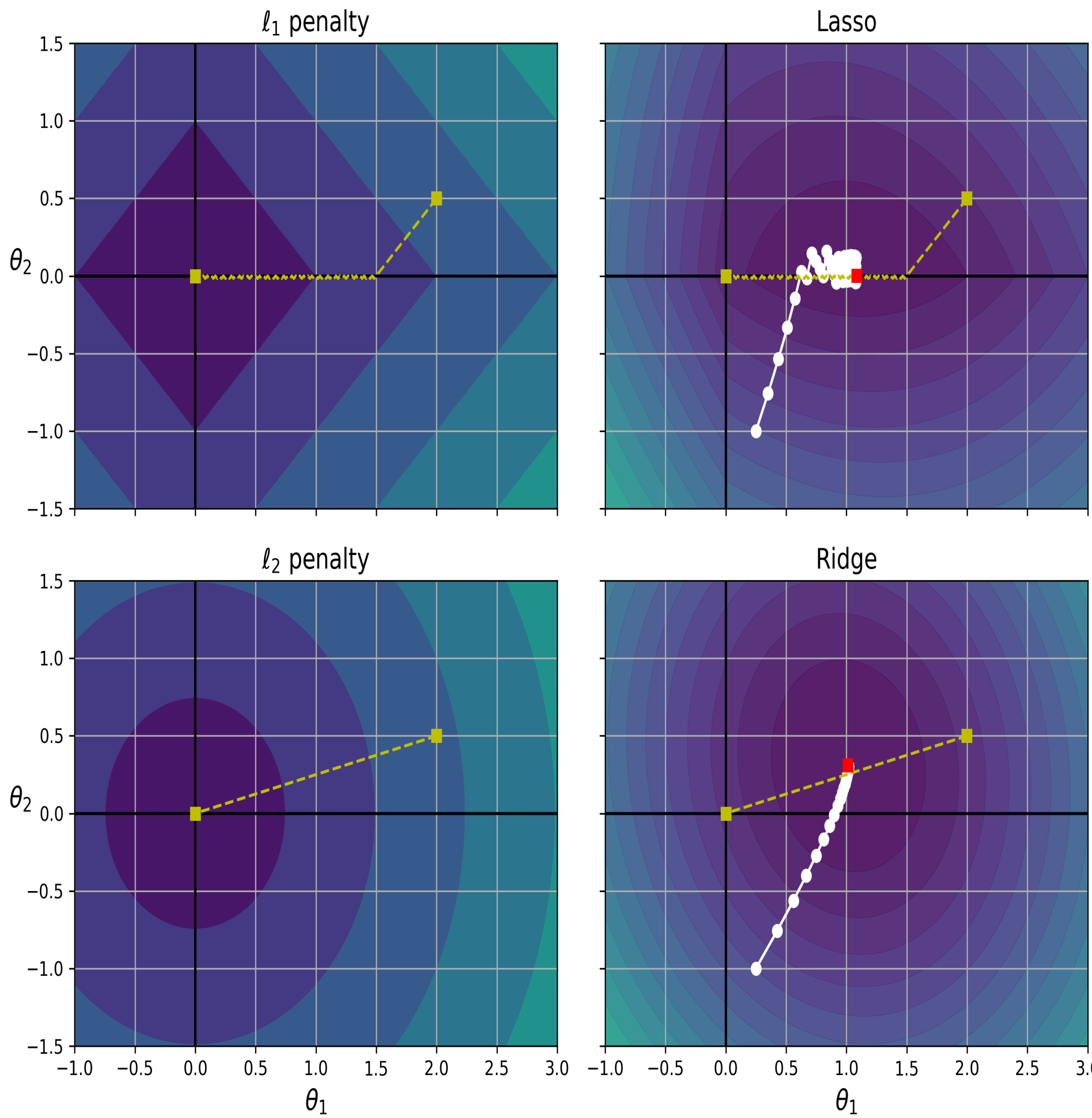


Figure 4-19. Lasso versus Ridge regularization

The two bottom plots show the same thing but with an ℓ_2 penalty instead. In the bottom-left plot, you can see that the ℓ_2 loss decreases as we get closer to the origin, so Gradient Descent just takes a straight path toward that point. In the bottom-right plot, the contours represent Ridge Regression's cost function (i.e., an MSE cost function plus an ℓ_2 loss). As you can see, the gradients get smaller as the parameters approach the global optimum, so Gradient Descent naturally slows down, which helps convergence (as there is no bouncing around). This helps Ridge converge faster than Lasso. Also note that the optimal parameters (represented by the red square) get closer and closer to the origin when you increase α, but they never get eliminated entirely.

TIP

To avoid Gradient Descent from bouncing around the optimum at the end when using Lasso, you need to gradually reduce the learning rate during training (it will still bounce around the optimum, but the steps will get smaller and smaller, so it will converge).

The Lasso cost function is not differentiable at $\theta_i = 0$ (for $i = 1, 2, \cdots, n$), but Gradient Descent still works fine if you use a *subgradient vector* **g**[11] instead when any $\theta_i = 0$. Equation 4-11 shows a subgradient vector equation you can use for Gradient Descent with the Lasso cost function.

Equation 4-11. Lasso Regression subgradient vector

$$g(\boldsymbol{\theta}, J) = \nabla_{\boldsymbol{\theta}}\, \mathrm{MSE}(\boldsymbol{\theta}) + 2\alpha \begin{pmatrix} \mathrm{sign}\,(\theta_1) \\ \mathrm{sign}\,(\theta_2) \\ \vdots \\ \mathrm{sign}\,(\theta_n) \end{pmatrix} \quad \text{where}\;\; \mathrm{sign}\,(\theta_i) = \begin{cases} -1 & \text{if } \theta_i < 0 \\ 0 & \text{if } \theta_i = 0 \\ +1 & \text{if } \theta_i > 0 \end{cases}$$

Here is a small Scikit-Learn example using the `Lasso` class:

```
>>> from sklearn.linear_model import Lasso
>>> lasso_reg = Lasso(alpha=0.1)
>>> lasso_reg.fit(X, y)
>>> lasso_reg.predict([[1.5]])
array([1.53788174])
```

Note that you could instead use `SGDRegressor(penalty="l1", alpha=0.1)`.

Elastic Net

Elastic Net is a middle ground between Ridge Regression and Lasso Regression. The regularization term is a weighted sum of both Ridge and Lasso's regularization terms, and you can control the mix ratio r. When $r = 0$, Elastic Net is equivalent to Ridge Regression, and when $r = 1$, it is equivalent to Lasso Regression (see Equation 4-12).

Equation 4-12. Elastic Net cost function

$$J(\boldsymbol{\theta}) = \mathrm{MSE}(\boldsymbol{\theta}) + r\left(2\alpha \sum_{i=1}^{n} |\theta_i|\right) + (1 - r)\left(\frac{\alpha}{m} \sum_{i=1}^{n} \theta_i^2\right)$$

So when should you use plain Linear Regression (i.e., without any regularization), Ridge, Lasso, or Elastic Net? It is almost always preferable to have at least a little bit of regularization, so generally you should avoid plain Linear Regression. Ridge is a good default, but if you suspect that only a few features are useful, you should prefer Lasso or Elastic Net because they tend to reduce the useless features' weights down to zero, as we have discussed. In general, Elastic Net is preferred over Lasso because Lasso may behave erratically when the number of features is greater than the number of training instances or when several features are strongly correlated.

Here is a short example that uses Scikit-Learn's `ElasticNet` (`l1_ratio` corresponds to the mix ratio r):

```
>>> from sklearn.linear_model import ElasticNet
>>> elastic_net = ElasticNet(alpha=0.1, l1_ratio=0.5)
>>> elastic_net.fit(X, y)
>>> elastic_net.predict([[1.5]])
array([1.54333232])
```

Early Stopping

A very different way to regularize iterative learning algorithms such as Gradient Descent is to stop training as soon as the validation error reaches a minimum. This is called *early stopping*. Figure 4-20 shows a complex model (in this case, a high-degree Polynomial Regression model) being trained with Batch Gradient Descent on the quadratic dataset we used earlier. As the epochs go by, the algorithm learns, and its prediction error (RMSE) on the training set goes down, along with its prediction error on the validation set. After a while though, the validation error stops decreasing and starts to go back up. This indicates that the model has started to overfit the training data. With early stopping you just stop training as soon as the validation error reaches the minimum. It is such a simple and efficient regularization technique that Geoffrey Hinton called it a "beautiful free lunch."

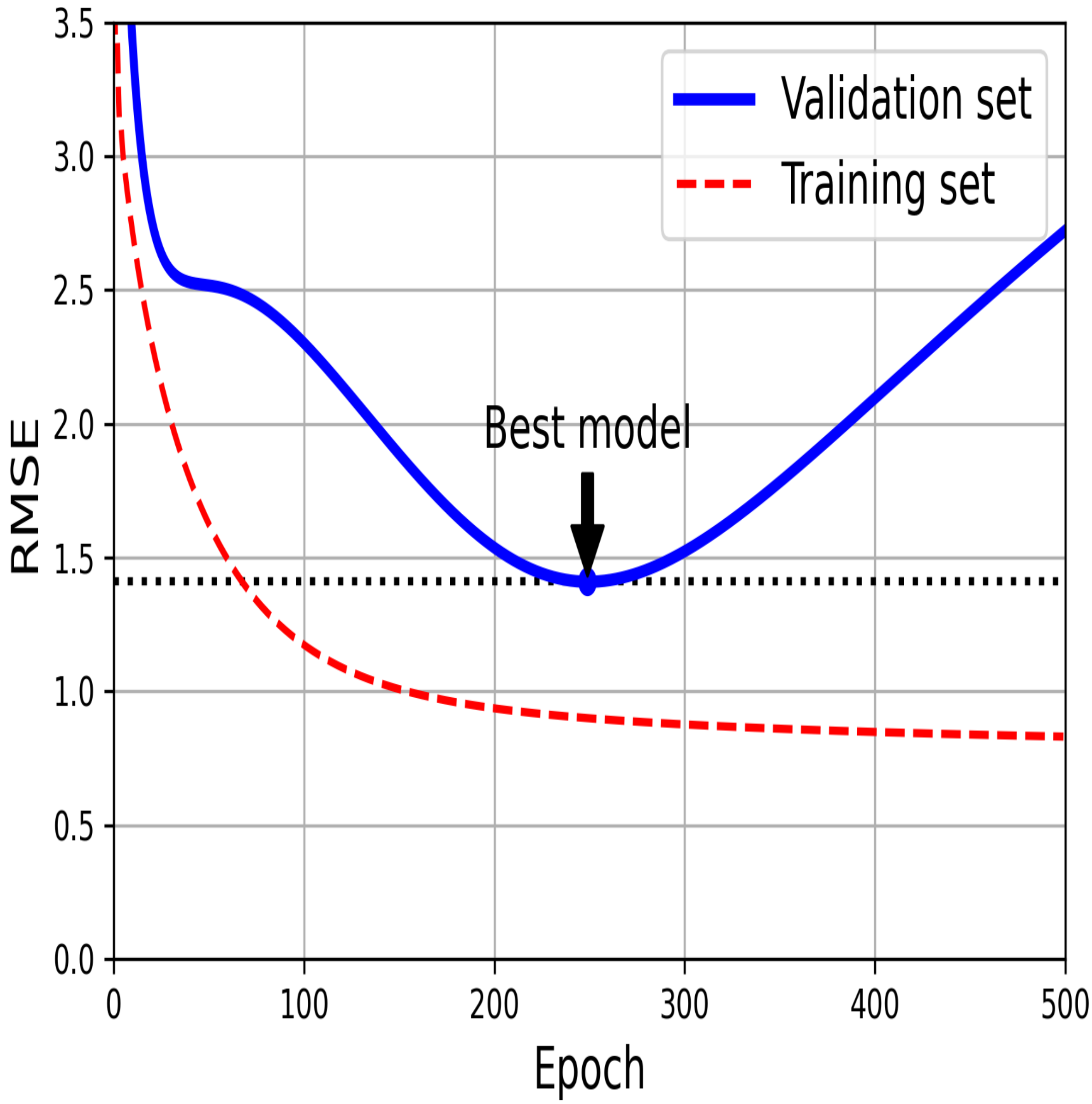


Figure 4-20. Early stopping regularization

> **TIP**
>
> With Stochastic and Mini-batch Gradient Descent, the curves are not so smooth, and it may be hard to know whether you have reached the minimum or not. One solution is to stop only after the validation error has been above the minimum for some time (when you are confident that the model will not do any better), then roll back the model parameters to the point where the validation error was at a minimum.

Here is a basic implementation of early stopping:

```
from copy import deepcopy
from sklearn.metrics import mean_squared_error
from sklearn.preprocessing import StandardScaler

X_train, y_train, X_valid, y_valid = [...]  # split the quadratic dataset

preprocessing = make_pipeline(PolynomialFeatures(degree=90, include_bias=False),
                              StandardScaler())
X_train_prep = preprocessing.fit_transform(X_train)
X_valid_prep = preprocessing.transform(X_valid)
sgd_reg = SGDRegressor(penalty=None, eta0=0.002, random_state=42)
n_epochs = 500
best_valid_rmse = float('inf')

for epoch in range(n_epochs):
    sgd_reg.partial_fit(X_train_prep, y_train)
    y_valid_predict = sgd_reg.predict(X_valid_prep)
    val_error = mean_squared_error(y_valid, y_valid_predict, squared=False)
    if val_error < best_valid_rmse:
        best_valid_rmse = val_error
        best_model = deepcopy(sgd_reg)
```

Here's what this code does: it first adds the polynomial features and scales all the input features, both for the training set and the validation set (this code assumes that you have split the training set into a smaller training set and a validation set). Then it creates an `SGDRegressor` model with no regularization and a small learning rate. In the training loop, it calls `partial_fit()` instead of `fit()`, to perform incremental learning. At each epoch, it measures the RMSE on the validation set. If it is lower than the lowest RMSE seen so far, it saves a copy of the model in the `best_model` variable. This implementation does not actually stop training, but it lets you revert to the best model after training. Note that the model is copied using `copy.deepcopy()`, because it copies both the model's hyperparameters *and* the learned parameters. In contrast, `sklearn.base.clone()` only copies the model's hyperparameters.

Logistic Regression

As we discussed in Chapter 1, some regression algorithms can be used for classification (and vice versa). *Logistic Regression* (also called *Logit Regression*) is commonly used to estimate the probability that an instance belongs to a particular class (e.g., what is the probability that this email is spam?). If the estimated probability is greater than a given threshold (typically 50%), then the model predicts that the instance belongs to that class (called the *positive class*, labeled "1"), and otherwise it predicts that it does not (i.e., it belongs to the *negative class*, labeled "0"). This makes it a binary classifier.

Estimating Probabilities

So how does Logistic Regression work? Just like a Linear Regression model, a Logistic Regression model computes a weighted sum of the input features (plus a bias term), but instead of outputting the result directly like the Linear Regression model does, it outputs the *logistic* of this result (see Equation 4-13).

Equation 4-13. Logistic Regression model estimated probability (vectorized form)

$$\widehat{p} = h_{\boldsymbol{\theta}}(\mathbf{x}) = \sigma\left(\boldsymbol{\theta}^{\intercal}\mathbf{x}\right)$$

The logistic—noted $\sigma(\cdot)$—is a *sigmoid function* (i.e., *S*-shaped) that outputs a number between 0 and 1. It is defined as shown in Equation 4-14 and Figure 4-21.

Equation 4-14. Logistic function

$$\sigma(t) = \frac{1}{1 + \exp(-t)}$$

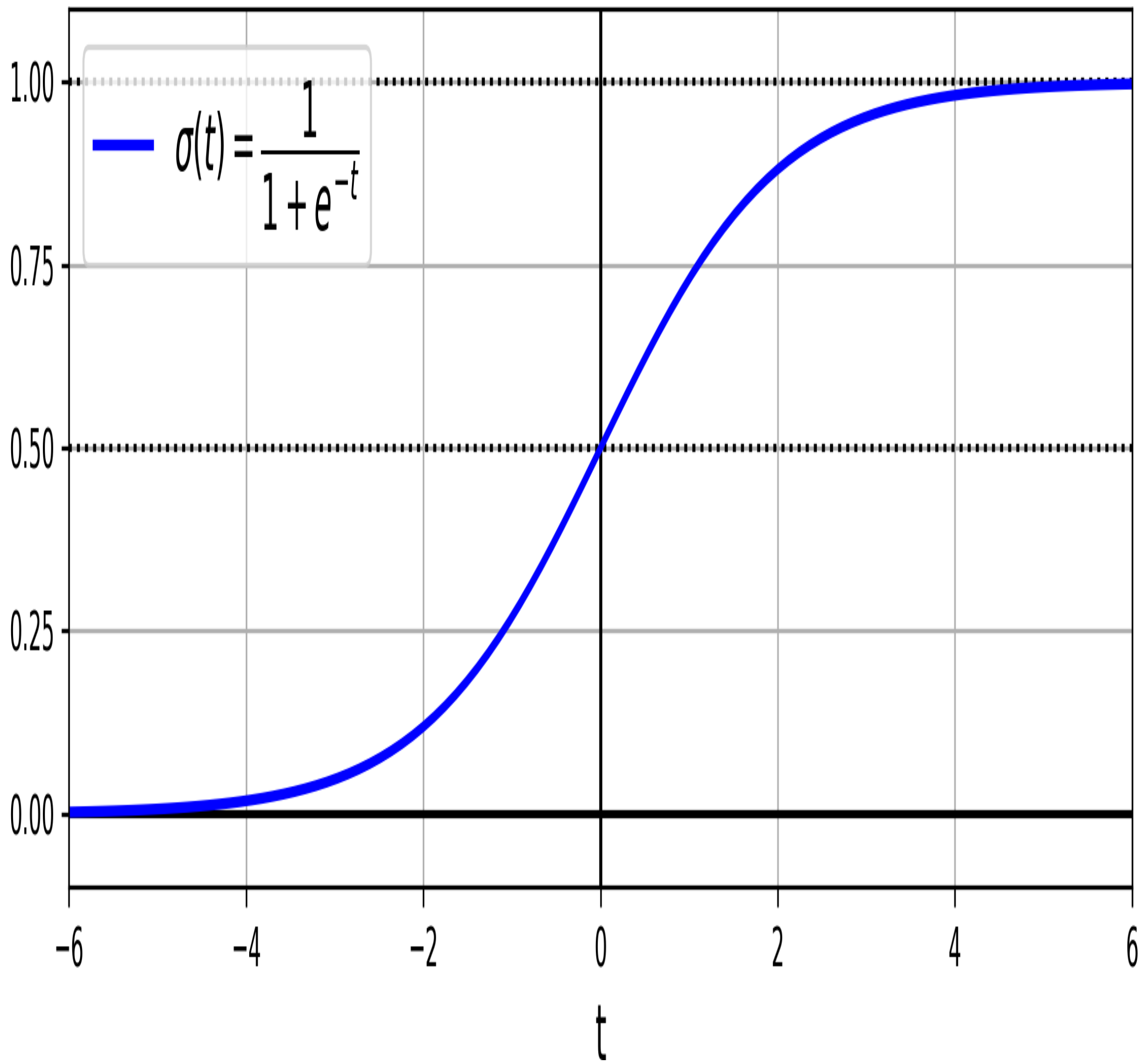


Figure 4-21. Logistic function

Once the Logistic Regression model has estimated the probability $\widehat{p} = h_{\boldsymbol{\theta}}(\mathbf{x})$ that an instance $\mathbf{x}$ belongs to the positive class, it can make its prediction $\hat{y}$ easily (see Equation 4-15).

Equation 4-15. Logistic Regression model prediction using a threshold probability of 50%

$$\hat{y} = \begin{cases} 0 & \text{if } \widehat{p} < 0.5 \\ 1 & \text{if } \widehat{p} \geq 0.5 \end{cases}$$

Notice that $\sigma(t) < 0.5$ when $t < 0$, and $\sigma(t) \geq 0.5$ when $t \geq 0$, so a Logistic Regression model using the default threshold of 50% probability predicts 1 if $\boldsymbol{\theta}^\intercal \mathbf{x}$ is positive and 0 if it is negative.

> **NOTE**
>
> The score t is often called the *logit*. The name comes from the fact that the logit function, defined as $\text{logit}(p) = \log(p / (1 - p))$, is the inverse of the logistic function. Indeed, if you compute the logit of the estimated probability p, you will find that the result is t. The logit is also called the *log-odds*, since it is the log of the ratio between the estimated probability for the positive class and the estimated probability for the negative class.

Training and Cost Function

Now you know how a Logistic Regression model estimates probabilities and makes predictions. But how is it trained? The objective of training is to set the parameter vector $\boldsymbol{\theta}$ so that the model estimates high probabilities for positive instances ($y = 1$) and low probabilities for negative instances ($y = 0$). This idea is captured by the cost function shown in Equation 4-16 for a single training instance $\mathbf{x}$.

Equation 4-16. Cost function of a single training instance

$$c(\boldsymbol{\theta}) = \begin{cases} -\log\left(\widehat{p}\right) & \text{if } y = 1 \\ -\log\left(1 - \widehat{p}\right) & \text{if } y = 0 \end{cases}$$

This cost function makes sense because $-\log(t)$ grows very large when t approaches 0, so the cost will be large if the model estimates a probability close to 0 for a positive instance, and it will also be very large if the model estimates a probability close to 1 for a negative instance. On the other hand, $-\log(t)$ is close to 0 when t is close to 1, so the cost will be close to 0 if the estimated probability is close to 0 for a negative instance or close to 1 for a positive instance, which is precisely what we want.

The cost function over the whole training set is the average cost over all training instances. It can be written in a single expression called the *log loss*, shown in Equation 4-17.

Equation 4-17. Logistic Regression cost function (log loss)

$$J(\boldsymbol{\theta}) = -\frac{1}{m} \sum_{i=1}^{m} \left[y^{(i)} log\left(\widehat{p}^{(i)}\right) + \left(1 - y^{(i)}\right) log\left(1 - \widehat{p}^{(i)}\right) \right]$$

> **WARNING**
>
> The log loss was not just pulled out of a hat. It can be shown mathematically (using Bayesian inference) that minimizing this loss will result in the model with the *maximum likelihood* of being optimal, assuming that the instances follow a Gaussian distribution around the mean of their class. When you use the log loss, this is the implicit assumption you are making. The more wrong this assumption is, the more biased the model will be. Similarly, when we used the MSE to train Linear Regression models, we were implicitly assuming that the data was purely linear, plus some Gaussian noise. So if the data is not linear (e.g., quadratic) or if the noise is not Gaussian (e.g., if outliers are not exponentially rare), then the model will be biased.

The bad news is that there is no known closed-form equation to compute the value of $\boldsymbol{\theta}$ that minimizes this cost function (there is no equivalent of the Normal Equation). But the good news is that this cost function is convex, so Gradient Descent (or any other optimization algorithm) is guaranteed to find the global minimum (if the learning rate is not too large and you wait long enough). The partial derivatives of the cost function with regard to the j^{th} model parameter θ_j are given by Equation 4-18.

Equation 4-18. Logistic cost function partial derivatives

$$\frac{\partial}{\partial \theta_j} \text{J}\left(\boldsymbol{\theta}\right) = \frac{1}{m} \sum_{i=1}^{m} \left(\sigma\left(\boldsymbol{\theta}^\intercal \mathbf{x}^{(i)}\right) - y^{(i)} \right) x_j^{(i)}$$

This equation looks very much like Equation 4-5: for each instance it computes the prediction error and multiplies it by the j^{th} feature value, and then it computes the average over all training instances. Once you have the gradient vector containing all the partial derivatives, you can use it in the Batch Gradient Descent algorithm. That's it: you now know how to train a Logistic Regression model. For Stochastic GD you would take one instance at a time, and for Mini-batch GD you would use a mini-batch at a time.

Decision Boundaries

Let's use the iris dataset to illustrate Logistic Regression. This is a famous dataset that contains the sepal and petal length and width of 150 iris flowers of three different species: *Iris setosa*, *Iris versicolor*, and *Iris virginica* (see Figure 4-22).

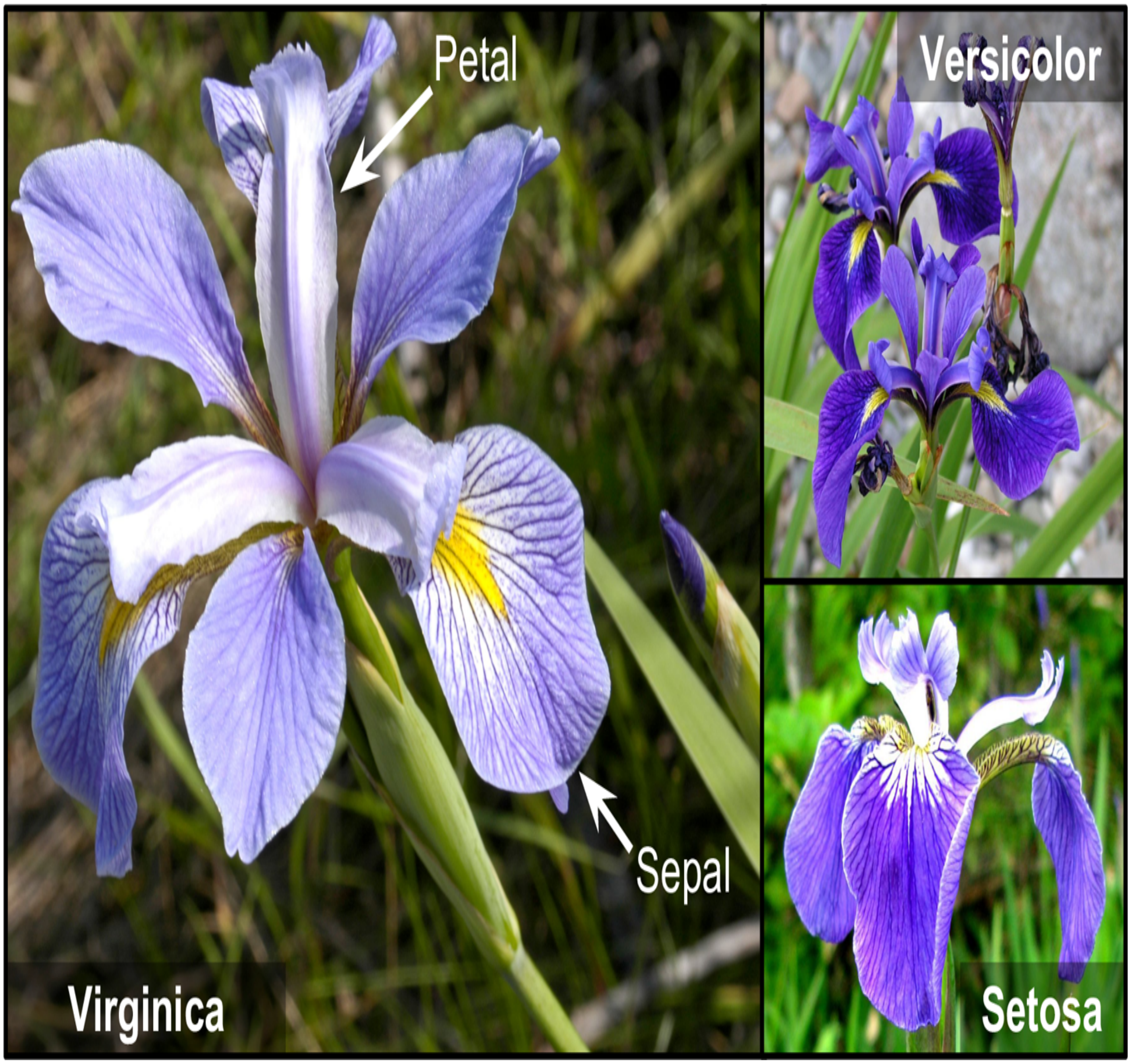


Figure 4-22. Flowers of three iris plant species[12]

Let's try to build a classifier to detect the *Iris virginica* type based only on the petal width feature. First let's load the data and take a quick peek:

```
>>> from sklearn.datasets import load_iris
>>> iris = load_iris(as_frame=True)
>>> list(iris)
```

```
['data', 'target', 'frame', 'target_names', 'DESCR', 'feature_names',
 'filename', 'data_module']
>>> iris.data.head(3)
   sepal length (cm)  sepal width (cm)  petal length (cm)  petal width (cm)
0                5.1               3.5                1.4               0.2
1                4.9               3.0                1.4               0.2
2                4.7               3.2                1.3               0.2
>>> iris.target.head(3)  # note that the instances are not shuffled
0    0
1    0
2    0
Name: target, dtype: int64
>>> iris.target_names
array(['setosa', 'versicolor', 'virginica'], dtype='<U10')
```

Now let's split the data and train a Logistic Regression model on the training set:

```
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import train_test_split

X = iris.data[["petal width (cm)"]].values
y = iris.target_names[iris.target] == 'virginica'
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=42)

log_reg = LogisticRegression(random_state=42)
log_reg.fit(X_train, y_train)
```

Let's look at the model's estimated probabilities for flowers with petal widths varying from 0 cm to 3 cm (Figure 4-23):[13]

```
X_new = np.linspace(0, 3, 1000).reshape(-1, 1)  # reshape to get a column vector
y_proba = log_reg.predict_proba(X_new)
decision_boundary = X_new[y_proba[:, 1] >= 0.5][0, 0]

plt.plot(X_new, y_proba[:, 0], "b--", linewidth=2,
         label="Not Iris virginica proba")
plt.plot(X_new, y_proba[:, 1], "g-", linewidth=2, label="Iris virginica proba")
plt.plot([decision_boundary, decision_boundary], [0, 1], "k:", linewidth=2,
         label="Decision boundary")
[...]  # beautify the figure: add grid, labels, axis, legend, arrows and samples
plt.show()
```

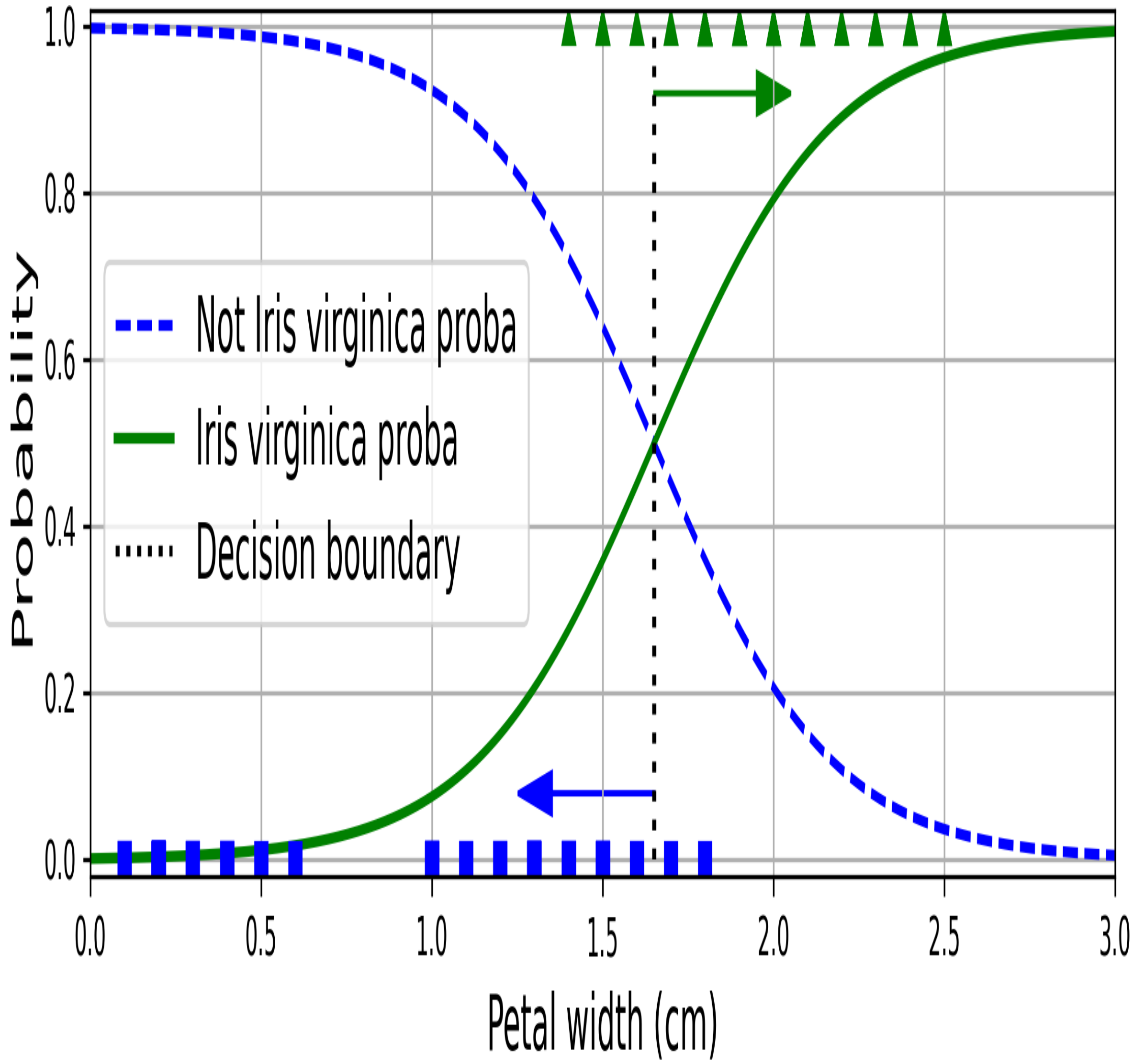


Figure 4-23. Estimated probabilities and decision boundary

The petal width of *Iris virginica* flowers (represented as triangles) ranges from 1.4 cm to 2.5 cm, while the other iris flowers (represented by squares) generally have a smaller petal width, ranging from 0.1 cm to 1.8 cm. Notice that there is a bit of overlap. Above about 2 cm the classifier is highly confident that the flower is an *Iris virginica* (it outputs a high probability for that class), while below 1 cm it is highly confident that it is not an *Iris virginica* (high probability for the "Not Iris virginica" class). In between these extremes, the classifier is unsure. However, if you ask it to predict the class (using the `predict()` method rather than the `predict_proba()` method), it will return whichever class is the most likely. Therefore, there is a *decision boundary* at around 1.6 cm where both probabilities are equal to 50%: if the petal width is higher than 1.6 cm, the classifier will predict that the flower is an *Iris virginica*, and otherwise it will predict that it is not (even if it is not very confident):

```
>>> decision_boundary
1.6516516516516517
>>> log_reg.predict([[1.7], [1.5]])
array([ True, False])
```

Figure 4-24 shows the same dataset, but this time displaying two features: petal width and length. Once trained, the Logistic Regression classifier can, based on these two features, estimate the probability that a new flower is an *Iris virginica*. The dashed line represents the points where the model estimates a 50% probability: this is the model's decision boundary. Note that it is a linear boundary.[14] Each parallel line represents the points where the model outputs a specific probability, from 15% (bottom left) to 90% (top right). All the flowers beyond the top-right line have over 90% chance of being *Iris virginica*, according to the model.

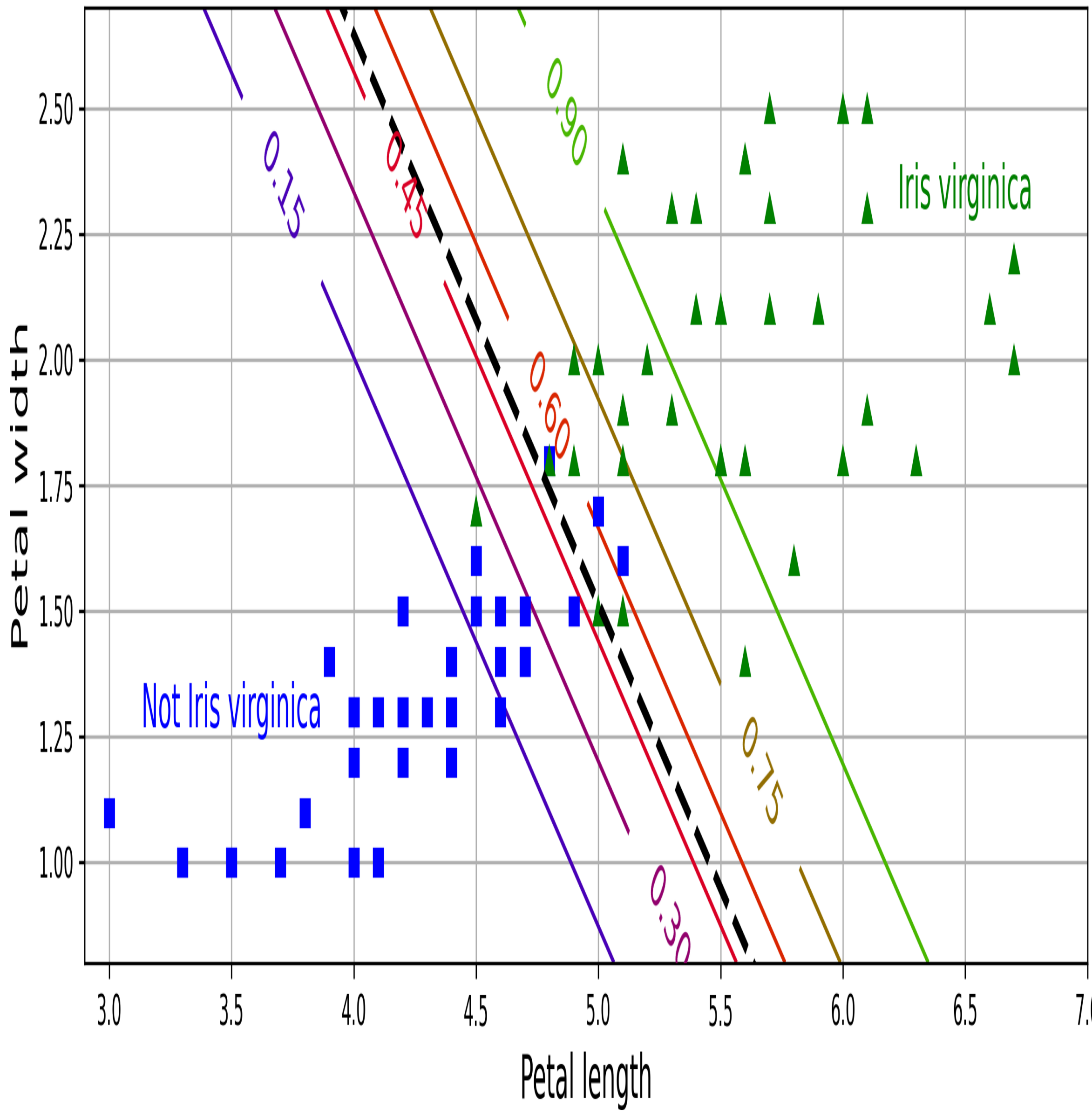


Figure 4-24. Linear decision boundary

Just like the other linear models, Logistic Regression models can be regularized using ℓ_1 or ℓ_2 penalties. Scikit-Learn actually adds an ℓ_2 penalty by default.

> **NOTE**
>
> The hyperparameter controlling the regularization strength of a Scikit-Learn `LogisticRegression` model is not `alpha` (as in other linear models), but its inverse: `C`. The higher the value of `C`, the *less* the model is regularized.

Softmax Regression

The Logistic Regression model can be generalized to support multiple classes directly, without having to train and combine multiple binary classifiers (as discussed in Chapter 3). This is called *Softmax Regression*, or *Multinomial Logistic Regression*.

The idea is simple: when given an instance $\mathbf{x}$, the Softmax Regression model first computes a score $s_k(\mathbf{x})$ for each class k, then estimates the probability of each class by applying the *softmax function* (also called the *normalized exponential*) to the scores. The equation to compute $s_k(\mathbf{x})$ should look familiar, as it is just like the equation for Linear Regression prediction (see Equation 4-19).

Equation 4-19. Softmax score for class k

$$s_k(\mathbf{x}) = \left(\boldsymbol{\theta}^{(k)}\right)^\intercal \mathbf{x}$$

Note that each class has its own dedicated parameter vector $\boldsymbol{\theta}^{(k)}$. All these vectors are typically stored as rows in a *parameter matrix* $\boldsymbol{\Theta}$.

Once you have computed the score of every class for the instance $\mathbf{x}$, you can estimate the probability $\widehat{p}_k$ that the instance belongs to class k by running the scores through the softmax function (Equation 4-20). The function computes the exponential of every score, then normalizes them (dividing by the sum of all the exponentials). The scores are generally called logits or log-odds (although they are actually unnormalized log-odds).

Equation 4-20. Softmax function

$$\widehat{p}_k = \sigma(\mathbf{s}(\mathbf{x}))_k = \frac{\exp\left(s_k(\mathbf{x})\right)}{\sum_{j=1}^{K} \exp\left(s_j(\mathbf{x})\right)}$$

In this equation:

- K is the number of classes.
- $\mathbf{s}(\mathbf{x})$ is a vector containing the scores of each class for the instance $\mathbf{x}$.
- $\sigma(\mathbf{s}(\mathbf{x}))_k$ is the estimated probability that the instance $\mathbf{x}$ belongs to class k, given the scores of each class for that instance.

Just like the Logistic Regression classifier, by default the Softmax Regression classifier predicts the class with the highest estimated probability (which is simply the class with the highest score), as shown in Equation 4-21.

Equation 4-21. Softmax Regression classifier prediction

$$\hat{y} = \underset{k}{\operatorname{argmax}}\ \sigma(\mathbf{s}(\mathbf{x}))_k = \underset{k}{\operatorname{argmax}}\ s_k(\mathbf{x}) = \underset{k}{\operatorname{argmax}}\ \left(\left(\boldsymbol{\theta}^{(k)}\right)^\intercal \mathbf{x}\right)$$

The *argmax* operator returns the value of a variable that maximizes a function. In this equation, it returns the value of k that maximizes the estimated probability $\sigma(\mathbf{s}(\mathbf{x}))_k$.

> **TIP**
>
> The Softmax Regression classifier predicts only one class at a time (i.e., it is multiclass, not multioutput), so it should be used only with mutually exclusive classes, such as different species of plants. You cannot use it to recognize multiple people in one picture.

Now that you know how the model estimates probabilities and makes predictions, let's take a look at training. The objective is to have a model that estimates a high probability for the target class (and consequently a low probability for the other classes). Minimizing the cost function shown in Equation 4-22, called the *cross entropy*, should lead to this objective because it penalizes the model when it estimates a low probability for a target class. Cross entropy is frequently used to measure how well a set of estimated class probabilities matches the target classes.

Equation 4-22. Cross entropy cost function

$$J(\boldsymbol{\Theta}) = -\frac{1}{m}\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} \log\left(\hat{p}_k^{(i)}\right)$$

In this equation:

- $y_k^{(i)}$ is the target probability that the i^{th} instance belongs to class k. In general, it is either equal to 1 or 0, depending on whether the instance belongs to the class or not.

Notice that when there are just two classes ($K = 2$), this cost function is equivalent to the Logistic Regression's cost function (log loss; see Equation 4-17).

CROSS ENTROPY

Cross entropy originated from Claude Shannon's *information theory*. Suppose you want to efficiently transmit information about the weather every day. If there are eight options (sunny, rainy, etc.), you could encode each option using three bits because $2^3 = 8$. However, if you think it will be sunny almost every day, it would be much more efficient to code "sunny" on just one bit (0) and the other seven options on four bits (starting with a 1). Cross entropy measures the average number of bits you actually send per option. If your assumption about the weather is perfect, cross entropy will be equal to the entropy of the weather itself (i.e., its intrinsic unpredictability). But if your assumptions are wrong (e.g., if it rains often), cross entropy will be greater by an amount called the *Kullback–Leibler (KL) divergence*.

The cross entropy between two probability distributions p and q is defined as $H(p,q) = -\Sigma_x\, p(x) \log q(x)$ (at least when the distributions are discrete). For more details, check out my video on the subject.

The gradient vector of this cost function with regard to $\boldsymbol{\theta}^{(k)}$ is given by Equation 4-23.

Equation 4-23. Cross entropy gradient vector for class k

$$\nabla_{\boldsymbol{\theta}^{(k)}}\, J(\boldsymbol{\Theta}) = \frac{1}{m}\sum_{i=1}^{m}\left(\hat{p}_k^{(i)} - y_k^{(i)}\right)\mathbf{x}^{(i)}$$

Now you can compute the gradient vector for every class, then use Gradient Descent (or any other optimization algorithm) to find the parameter matrix $\boldsymbol{\Theta}$ that minimizes the cost function.

Let's use Softmax Regression to classify the iris plants into all three classes. Scikit-Learn's `LogisticRegression` uses Softmax Regression automatically when you train it on more than two classes (assuming you use `solver="lbfgs"`, which is the default). It also applies ℓ_2 regularization by default, which you can control using the hyperparameter `C`, as earlier:

```
X = iris.data[["petal length (cm)", "petal width (cm)"]].values
y = iris["target"]
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=42)

softmax_reg = LogisticRegression(C=30, random_state=42)
softmax_reg.fit(X_train, y_train)
```

So the next time you find an iris with petals that are 5 cm long and 2 cm wide, you can ask your model to tell you what type of iris it is, and it will answer *Iris virginica* (class 2) with 96% probability (or *Iris versicolor* with 4% probability):

```
>>> softmax_reg.predict([[5, 2]])
array([2])
>>> softmax_reg.predict_proba([[5, 2]]).round(2)
array([[0.  , 0.04, 0.96]])
```

Figure 4-25 shows the resulting decision boundaries, represented by the background colors. Notice that the decision boundaries between any two classes are linear. The figure also shows the probabilities for the *Iris versicolor* class, represented by the curved lines (e.g., the line labeled with 0.30 represents the 30% probability boundary). Notice that the model can predict a class that has an estimated probability below 50%. For example, at the point where all decision boundaries meet, all classes have an equal estimated probability of 33%.

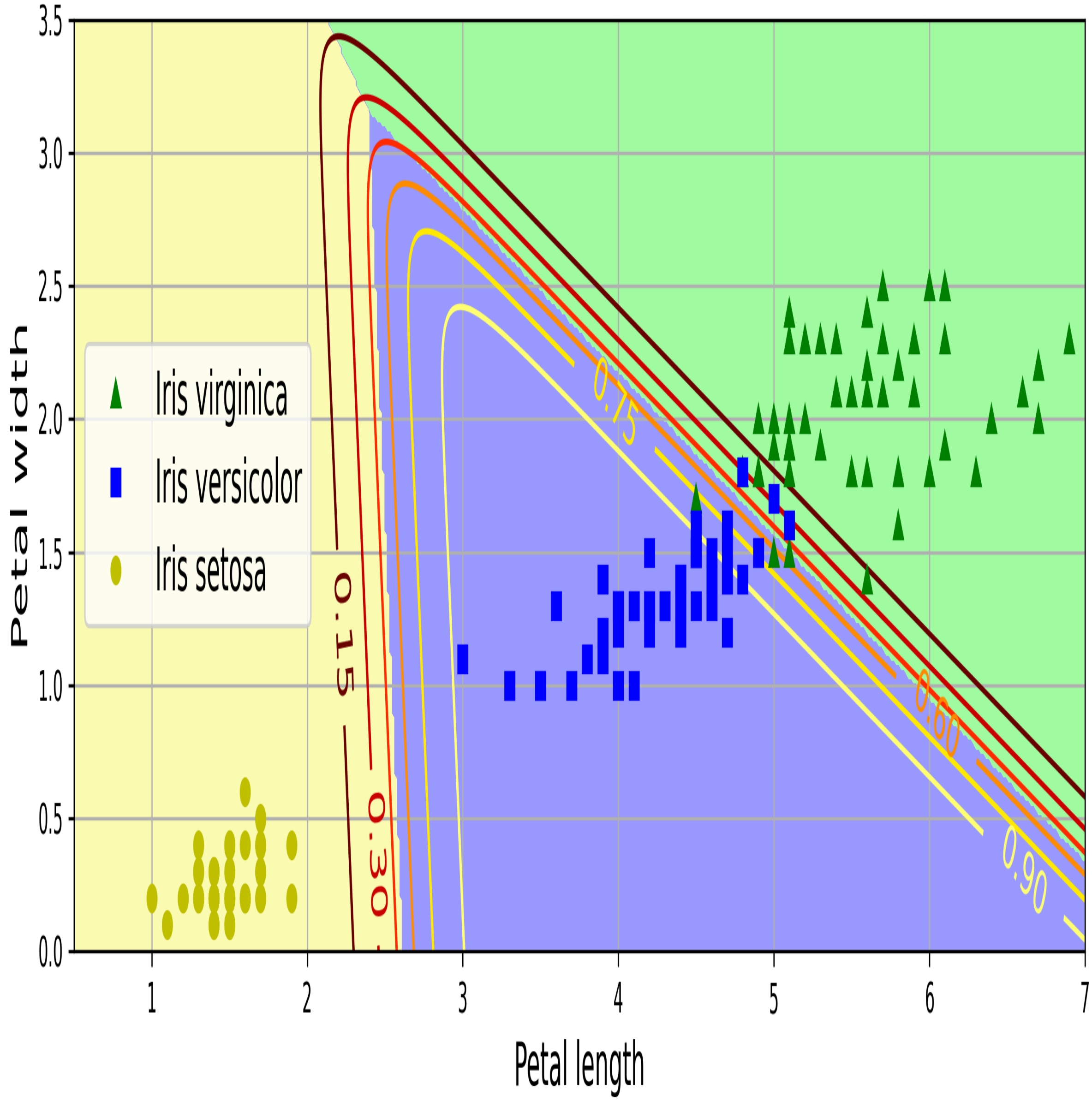


Figure 4-25. Softmax Regression decision boundaries

In this chapter, you learned various ways to train linear models, both for regression and classification. You used a closed-form equation to solve Linear Regression, as well as Gradient Descent, and you learned how various penalties can be added to the cost function during training to regularize the model. Along the way, you also learned how to plot learning curves and analyze them, and how to implement early stopping. Finally, you learned how Logistic Regression and Softmax Regression work. We've opened up the first Machine Learning black boxes! In the next chapters, we will open many more, starting with Decision Trees.

Exercises

1. Which Linear Regression training algorithm can you use if you have a training set with millions of features?
2. Suppose the features in your training set have very different scales. Which algorithms might suffer from this, and how? What can you do about it?
3. Can Gradient Descent get stuck in a local minimum when training a Logistic Regression model?
4. Do all Gradient Descent algorithms lead to the same model, provided you let them run long enough?
5. Suppose you use Batch Gradient Descent and you plot the validation error at every epoch. If you notice that the validation error consistently goes up, what is likely going on? How can you fix this?
6. Is it a good idea to stop Mini-batch Gradient Descent immediately when the validation error goes up?
7. Which Gradient Descent algorithm (among those we discussed) will reach the vicinity of the optimal solution the fastest? Which will actually converge? How can you make the others converge as well?
8. Suppose you are using Polynomial Regression. You plot the learning curves and you notice that there is a large gap between the training error and the validation error. What is happening? What are three ways to solve this?
9. Suppose you are using Ridge Regression and you notice that the training error and the validation error are almost equal and fairly high. Would you say that the model suffers from high bias or high variance? Should you increase the regularization hyperparameter α or reduce it?
10. Why would you want to use:
    a. Ridge Regression instead of plain Linear Regression (i.e., without any regularization)?
    b. Lasso instead of Ridge Regression?
    c. Elastic Net instead of Lasso?
11. Suppose you want to classify pictures as outdoor/indoor and daytime/nighttime. Should you implement two Logistic Regression classifiers or one Softmax Regression classifier?
12. Implement Batch Gradient Descent with early stopping for Softmax Regression without using Scikit-Learn, only NumPy. Use it on a classification task such as the iris dataset.

Solutions to these exercises are available at the end of this chapter's notebook, at *https://homl.info/colab3*.

---

1 Technically speaking, its derivative is *Lipschitz continuous*.

2 Since feature 1 is smaller, it takes a larger change in θ_1 to affect the cost function, which is why the bowl is elongated along the θ_1 axis.

3 Eta (η) is the seventh letter of the Greek alphabet.

4 While the Normal Equation can only perform Linear Regression, the Gradient Descent algorithms can be used to train many other models, as we will see.

5 A quadratic equation is of the form $y = ax^2 + bx + c$.

6 This notion of bias is not to be confused with the bias term of linear models.

7 It is common to use the notation $J(\boldsymbol{\theta})$ for cost functions that don't have a short name; we will often use this notation throughout the rest of this book. The context will make it clear which cost function is being discussed.

8 Norms are discussed in Chapter 2.

9 A square matrix full of 0s except for 1s on the main diagonal (top left to bottom right).

10 Alternatively you can use the `Ridge` class with the `"sag"` solver. Stochastic Average GD is a variant of Stochastic GD. For more details, see the presentation "Minimizing Finite Sums with the Stochastic Average Gradient Algorithm" by Mark Schmidt et al. from the University of British Columbia.

11 You can think of a subgradient vector at a nondifferentiable point as an intermediate vector between the gradient vectors around that point.

12 Photos reproduced from the corresponding Wikipedia pages. *Iris virginica* photo by Frank Mayfield (Creative Commons BY-SA 2.0), *Iris versicolor* photo by D. Gordon E. Robertson (Creative Commons BY-SA 3.0), *Iris setosa* photo public domain.

13 NumPy's `reshape()` function allows one dimension to be –1, which means "automatic": the value is inferred from the length of the array and the remaining dimensions.

14 It is the the set of points $\mathbf{x}$ such that $\theta_0 + \theta_1 x_1 + \theta_2 x_2 = 0$, which defines a straight line.

Chapter 5. Support Vector Machines

A NOTE FOR EARLY RELEASE READERS

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.

This will be the 5th chapter of the final book. Notebooks are available on GitHub at *https://github.com/ageron/handson-ml3*. Datasets are available at *https://github.com/ageron/data*.

If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the editoor at ntache@oreilly.com.

A *Support Vector Machine* (SVM) is a powerful and versatile Machine Learning model, capable of performing linear or nonlinear classification, regression, and even novelty detection. SVMs shine with small to medium-sized nonlinear datasets (i.e., hundreds to thousands of instances), especially for classification tasks. However, they don't scale very well to very large datasets, as we will see.

This chapter will explain the core concepts of SVMs, how to use them, and how they work. Let's jump right in!

Linear SVM Classification

The fundamental idea behind SVMs is best explained with some pictures. Figure 5-1 shows part of the iris dataset that was introduced at the end of Chapter 4. The two classes can clearly be separated easily with a straight line (they are *linearly separable*). The left plot shows the decision boundaries of three possible linear classifiers. The model whose decision boundary is represented by the dashed line is so bad that it does not even separate the classes properly. The other two models work perfectly on this training set, but their decision boundaries come so close to the instances that these models will probably not perform as well on new instances. In contrast, the solid line in the plot on the right represents the decision boundary of an SVM classifier; this line not only separates the two classes but also stays as far away from the closest training instances as possible. You can think of an SVM classifier as fitting the widest possible street (represented by the parallel dashed lines) between the classes. This is called *large margin classification*.

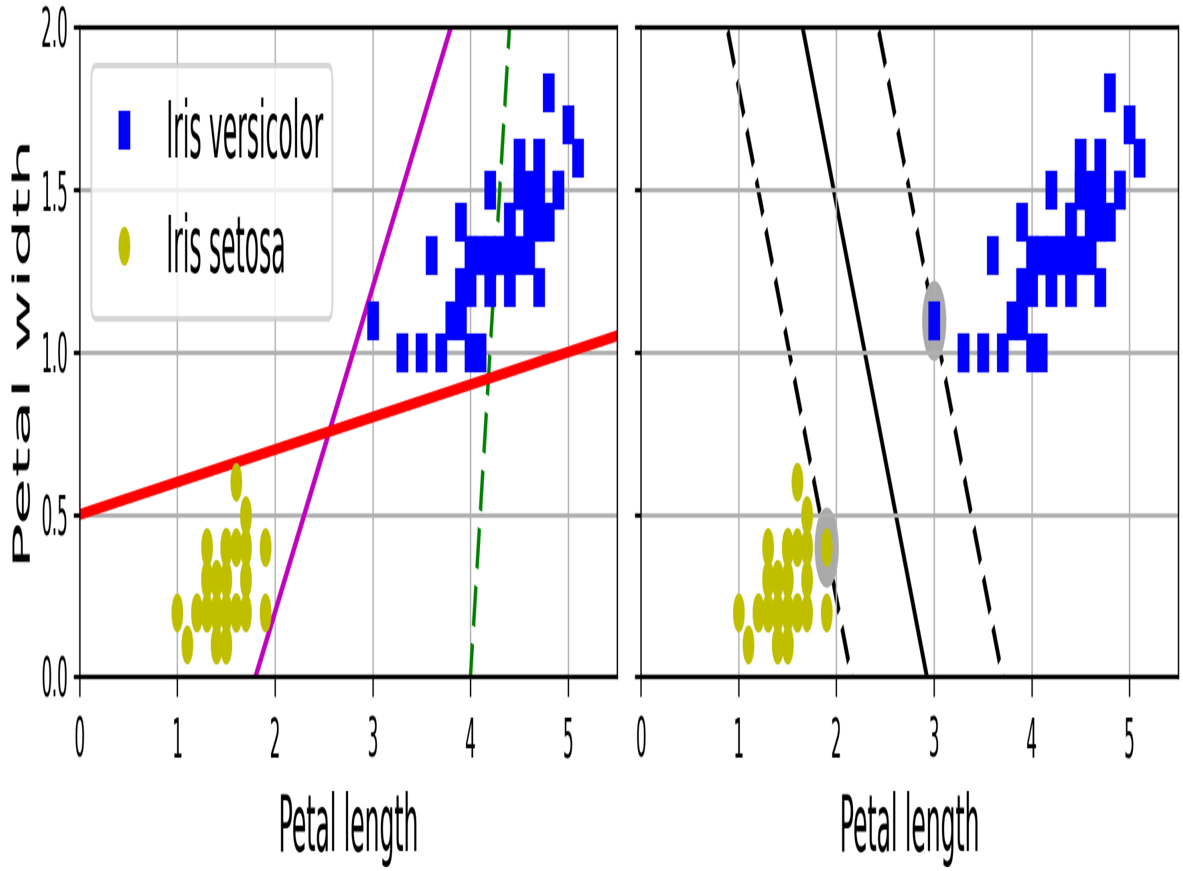


Figure 5-1. Large margin classification

Notice that adding more training instances "off the street" will not affect the decision boundary at all: it is fully determined (or "supported") by the instances located on the edge of the street. These instances are called the *support vectors* (they are circled in Figure 5-1).

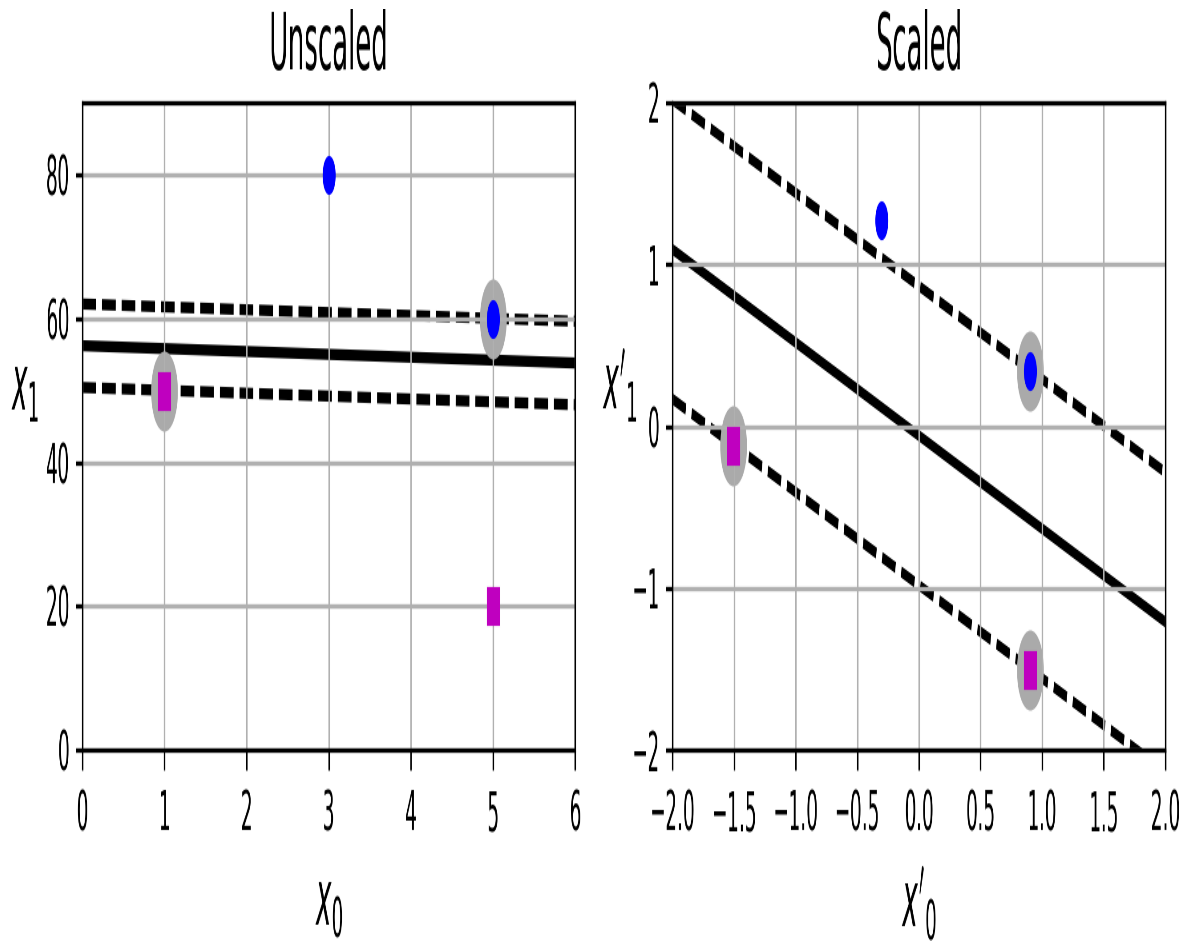


Figure 5-2. Sensitivity to feature scales

WARNING

SVMs are sensitive to the feature scales, as you can see in Figure 5-2: in the left plot, the vertical scale is much larger than the horizontal scale, so the widest possible street is close to horizontal. After feature scaling (e.g., using Scikit-Learn's `StandardScaler`), the decision boundary in the right plot looks much better.

Soft Margin Classification

If we strictly impose that all instances must be off the street and on the correct side, this is called *hard margin classification*. There are two main issues with hard margin classification. First, it only works if the data is linearly separable. Second, it is sensitive to outliers. Figure 5-3 shows the iris dataset with just one additional outlier: on the left, it is impossible to find a hard margin; on the right, the decision boundary ends up very different from the one we saw in Figure 5-1 without the outlier, and it will probably not generalize as well.

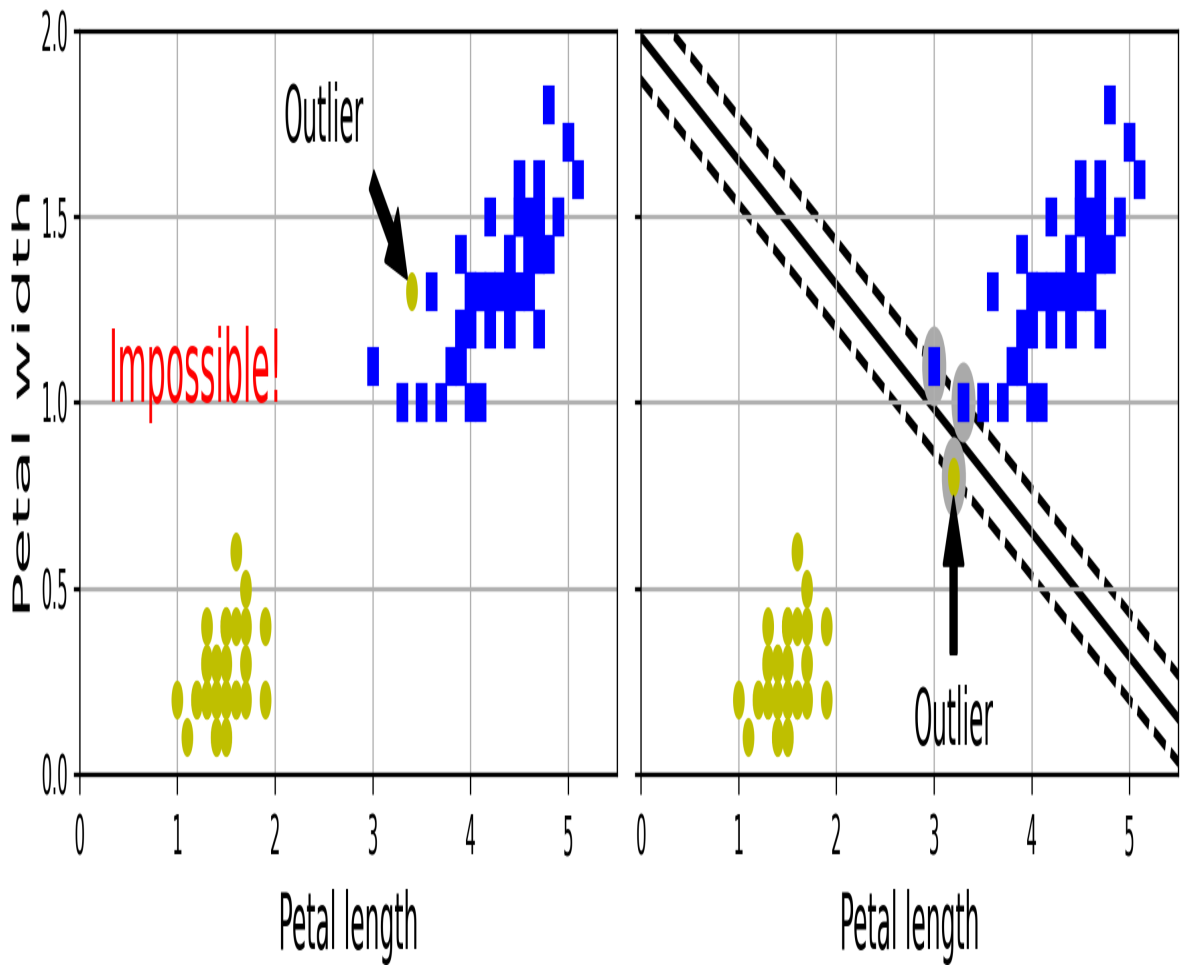


Figure 5-3. Hard margin sensitivity to outliers

To avoid these issues, use a more flexible model. The objective is to find a good balance between keeping the street as large as possible and limiting the *margin violations* (i.e., instances that end up in the middle of the street or even on the wrong side). This is called *soft margin classification*.

When creating an SVM model using Scikit-Learn, you can specify several hyperparameters, including a regularization hyperparameter called `C`. If you set it to a low value, then you end up with the model on the left of Figure 5-4. With a high value, you get the model on the right. As you can see, reducing `C` makes the street larger, but it also leads to more margin violations. In other words, reducing `C` results in more instances supporting the street, so there's less risk of overfitting. But if you reduce it too much, then the model ends up underfitting, as seems to be the case here: the model with `C=100` looks like it will generalize better than the one with `C=1`.

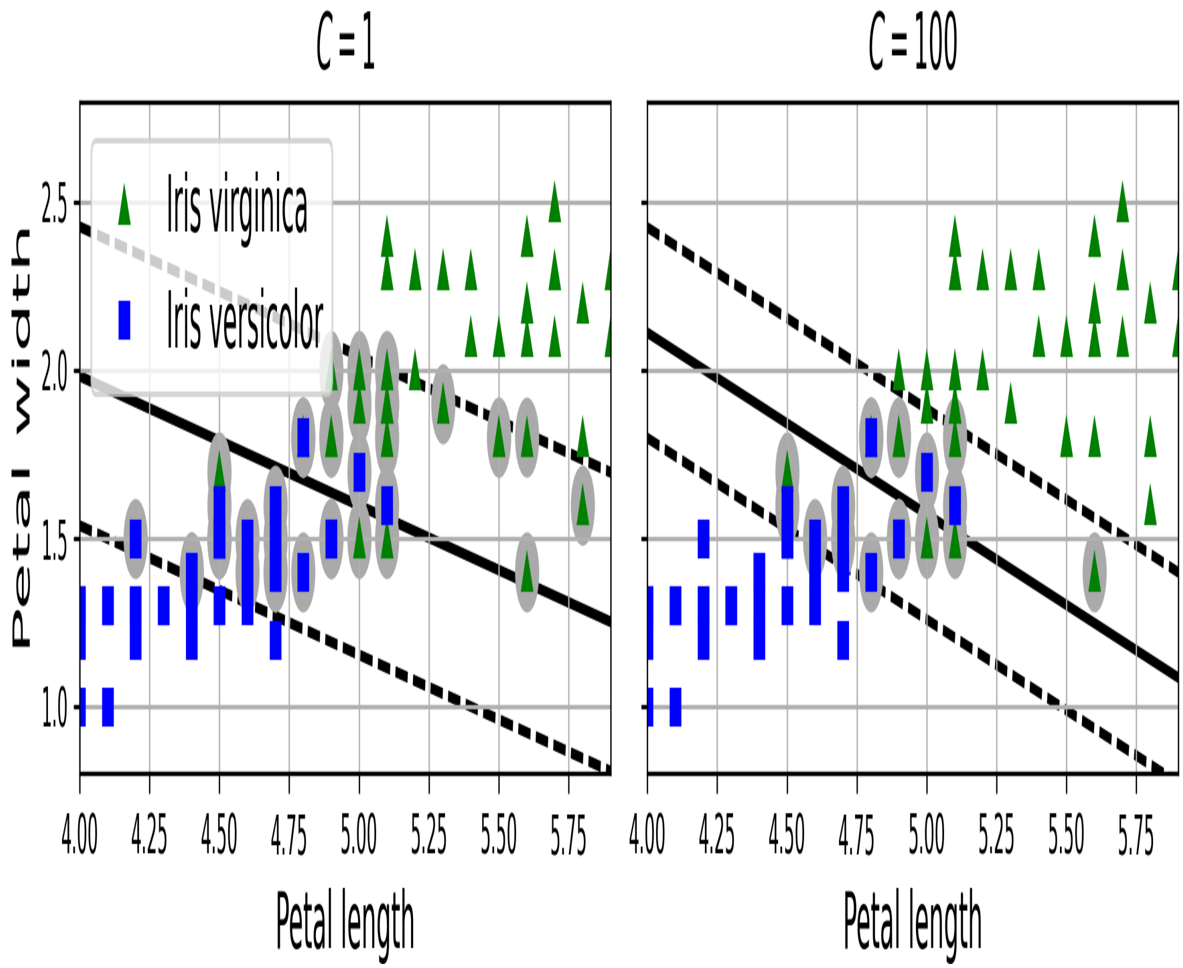


Figure 5-4. Large margin (left) versus fewer margin violations (right)

> **TIP**
>
> If your SVM model is overfitting, you can try regularizing it by reducing `C`.

The following Scikit-Learn code loads the iris dataset, and trains a linear SVM classifier to detect *Iris virginica* flowers. The pipeline first scales the features, then uses a `LinearSVC` with `C=1`:

```
from sklearn.datasets import load_iris
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.svm import LinearSVC

iris = load_iris(as_frame=True)
X = iris.data[["petal length (cm)", "petal width (cm)"]].values
y = (iris.target == 2)  # Iris virginica

svm_clf = make_pipeline(StandardScaler(),
                        LinearSVC(C=1, random_state=42))
svm_clf.fit(X, y)
```

The resulting model is represented on the left in Figure 5-4.

Then, as usual, you can use the model to make predictions:

```
>>> X_new = [[5.5, 1.7], [5.0, 1.5]]
>>> svm_clf.predict(X_new)
array([ True, False])
```

The first plant is classified as an Iris virginia, while the second is not. Let's look at the scores that the SVM used to make these predictions. These measure the signed distance between each instance and the decision boundary:

```
>>> svm_clf.decision_function(X_new)
array([ 0.66163411, -0.22036063])
```

Unlike the `LogisticRegression` classifier, `LinearSVC` does not have a `predict_proba()` method to estimate the class probabilities. That said, if you use the `SVC` class (discussed shortly) instead of `LinearSVC`, and if you set its `probability` to `True`, then the model will fit an extra model at the end of training to map the SVM decision function scores to estimated probabilities. Under the hood, this requires using 5-fold cross-validation to generate out-of-sample predictions for every instance in the training set, then training a `LogisticRegression` model, so it will slow down training considerably. After that, the `predict_proba()` and `predict_log_proba()` methods will be available.

Nonlinear SVM Classification

Although linear SVM classifiers are efficient and often work surprisingly well, many datasets are not even close to being linearly separable. One approach to handling nonlinear datasets is to add more features, such as polynomial features (as you did in Chapter 4); in some cases this can result in a linearly separable dataset. Consider the left plot in Figure 5-5: it represents a simple dataset with just one feature, x_1. This dataset is not linearly separable, as you can see. But if you add a second feature $x_2 = (x_1)^2$, the resulting 2D dataset is perfectly linearly separable.

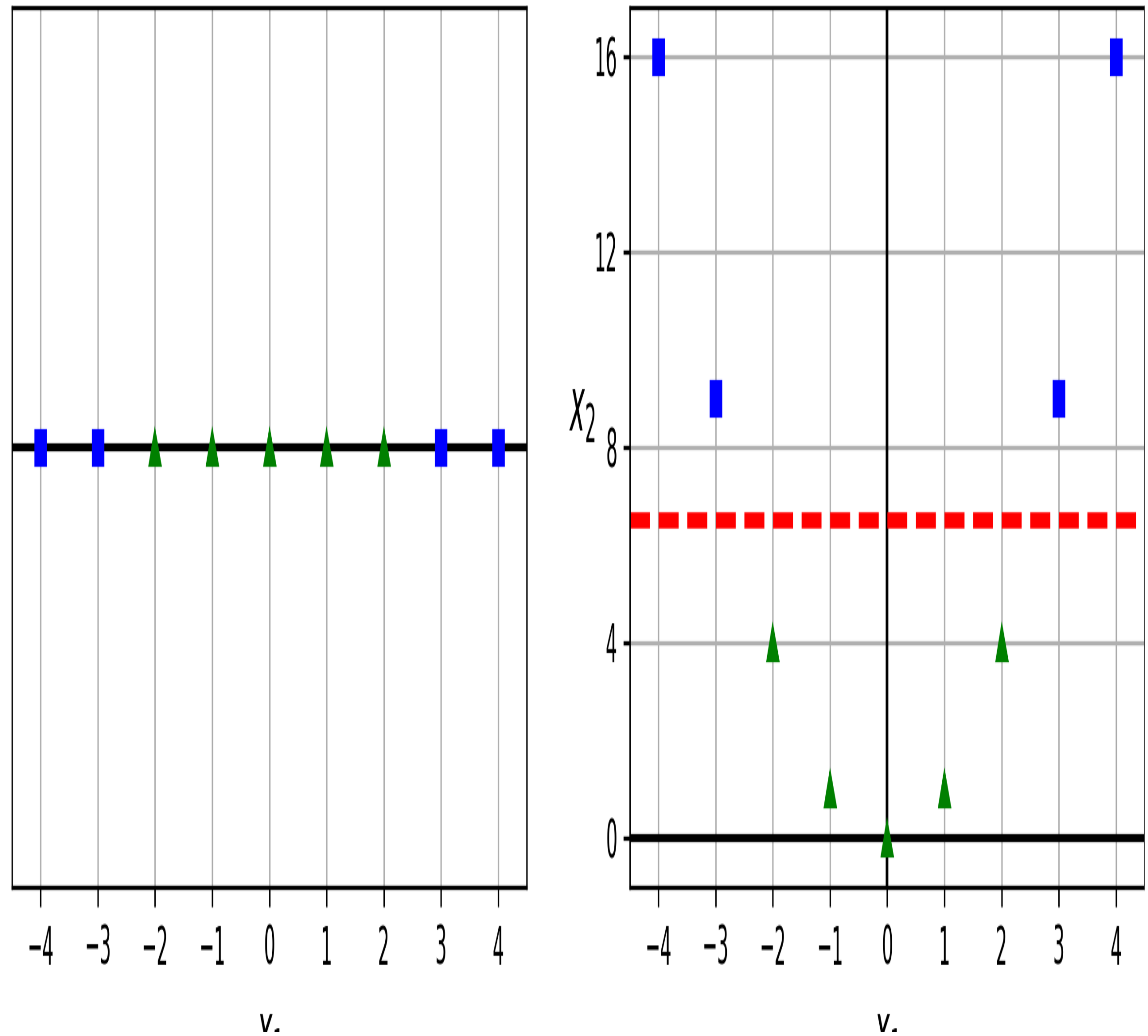


Figure 5-5. Adding features to make a dataset linearly separable

To implement this idea using Scikit-Learn, create a pipeline containing a `PolynomialFeatures` transformer (discussed in "Polynomial Regression"), followed by a `StandardScaler` and a `LinearSVC`. Let's test this on the moons dataset: this is a toy dataset for binary classification in which the data points are shaped as two interleaving crescent moons (see Figure 5-6). You can generate this dataset using the `make_moons()` function:

```
from sklearn.datasets import make_moons
from sklearn.preprocessing import PolynomialFeatures

X, y = make_moons(n_samples=100, noise=0.15, random_state=42)

polynomial_svm_clf = make_pipeline(
    PolynomialFeatures(degree=3),
    StandardScaler(),
    LinearSVC(C=10, max_iter=10_000, random_state=42)
)
polynomial_svm_clf.fit(X, y)
```

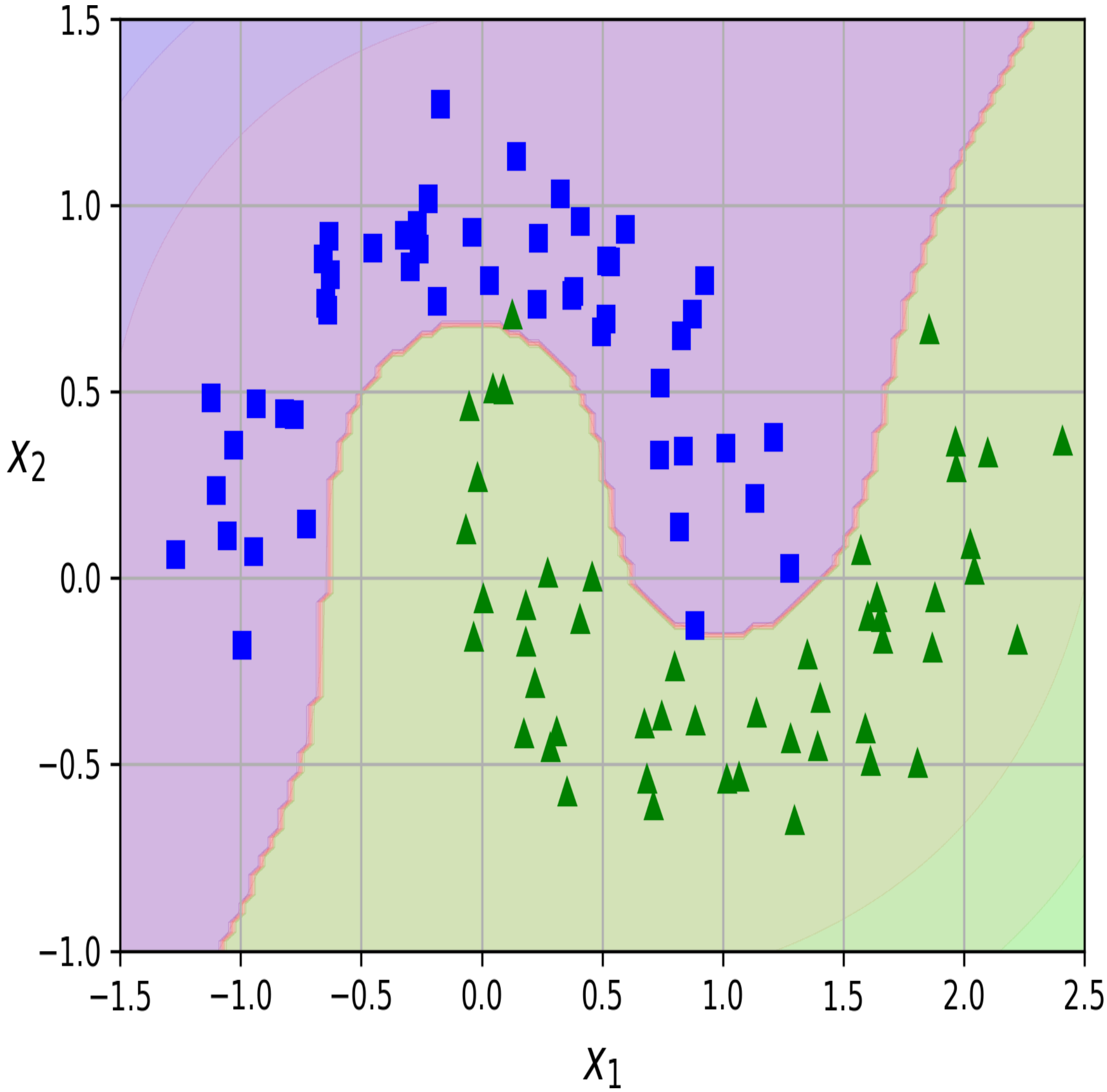


Figure 5-6. Linear SVM classifier using polynomial features

Polynomial Kernel

Adding polynomial features is simple to implement and can work great with all sorts of Machine Learning algorithms (not just SVMs). That said, at a low polynomial degree, this method cannot deal with very complex datasets, and with a high polynomial degree it creates a huge number of features, making the model too slow.

Fortunately, when using SVMs you can apply an almost miraculous mathematical technique called the *kernel trick* (which is explained later in this chapter). The kernel trick makes it possible to get the same result as if you had added many polynomial features, even with a very high-degree, without actually having to actually add them. This means there's no combinatorial explosion of the number of features. This trick is implemented by the `SVC` class. Let's test it on the moons dataset:

```
from sklearn.svm import SVC

poly_kernel_svm_clf = make_pipeline(StandardScaler(),
                                    SVC(kernel="poly", degree=3, coef0=1, C=5))
poly_kernel_svm_clf.fit(X, y)
```

This code trains an SVM classifier using a third-degree polynomial kernel. It is represented on the left in Figure 5-7. On the right is another SVM classifier using a 10th-degree polynomial kernel. Obviously, if your model is overfitting, you might want to reduce the polynomial degree. Conversely, if it is underfitting, you can try increasing it. The hyperparameter `coef0` controls how much the model is influenced by high-degree terms versus low-degree terms.

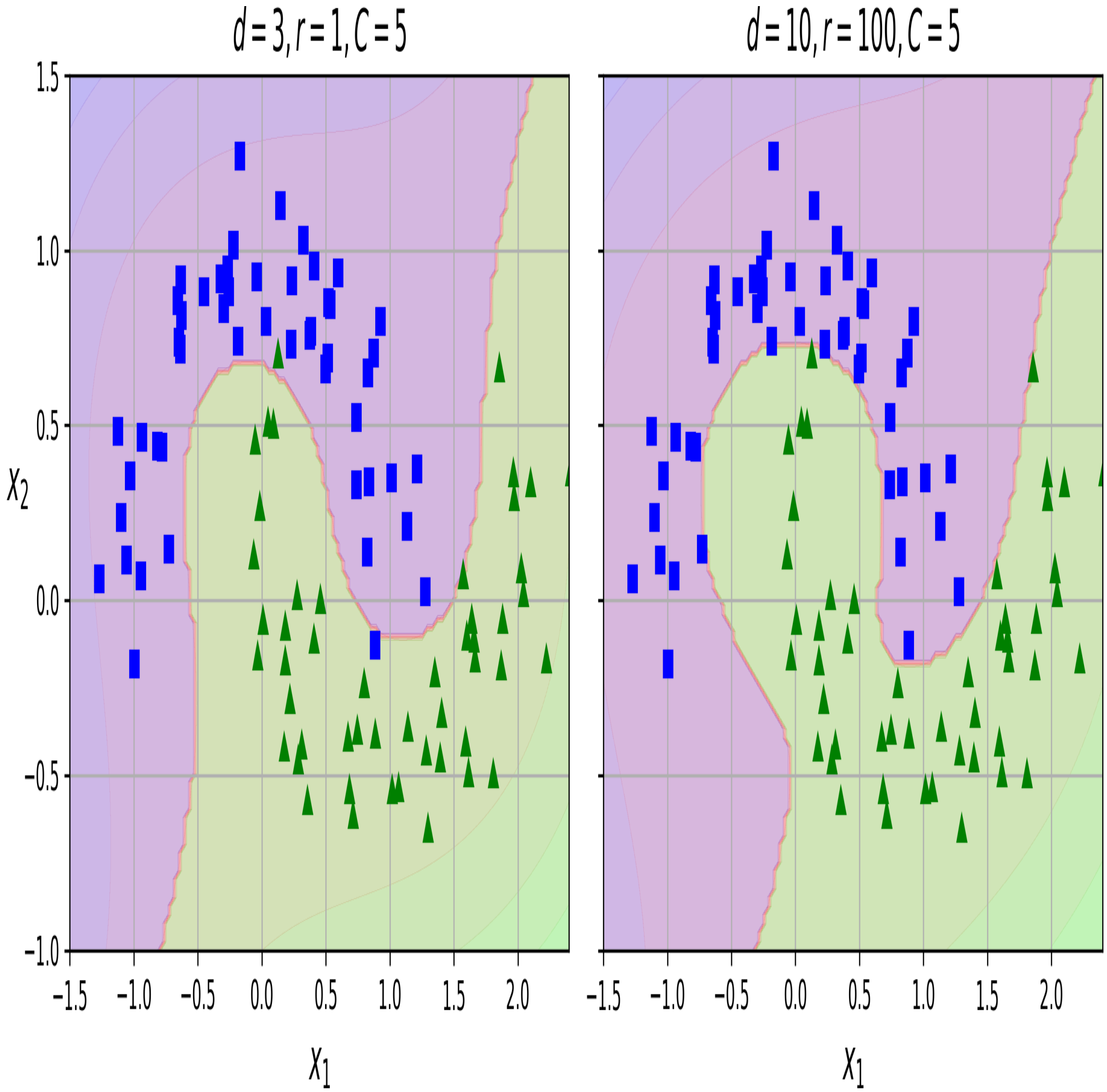


Figure 5-7. SVM classifiers with a polynomial kernel

> **TIP**
>
> Although you will typically tune hyperparameters automatically (e.g., using randomized search), it's good to have a sense of what each hyperparameter actually does, and how it may interact with other hyperparameters: this way, you can narrow the search to a much smaller space.

Similarity Features

Another technique to tackle nonlinear problems is to add features computed using a similarity function, which measures how much each instance resembles a particular *landmark*, as we did in Chapter 2 when we added the geographic similarity features. For example, let's take the 1D dataset discussed earlier and add two landmarks to it at $x_1 = –2$ and $x_1 = 1$ (see the left plot in Figure 5-8). Next, let's define the similarity function to be the Gaussian RBF with $\gamma = 0.3$. This is a bell-shaped function varying from 0 (very far away from the landmark) to 1 (at the landmark).

Now we are ready to compute the new features. For example, let's look at the instance $x_1 = –1$: it is located at a distance of 1 from the first landmark and 2 from the second landmark. Therefore its new features are $x_2 = \exp(–0.3 \times 1^2) \approx 0.74$ and $x_3 = \exp(–0.3 \times 2^2) \approx 0.30$. The plot on the right in Figure 5-8 shows the transformed dataset (dropping the original features). As you can see, it is now linearly separable.

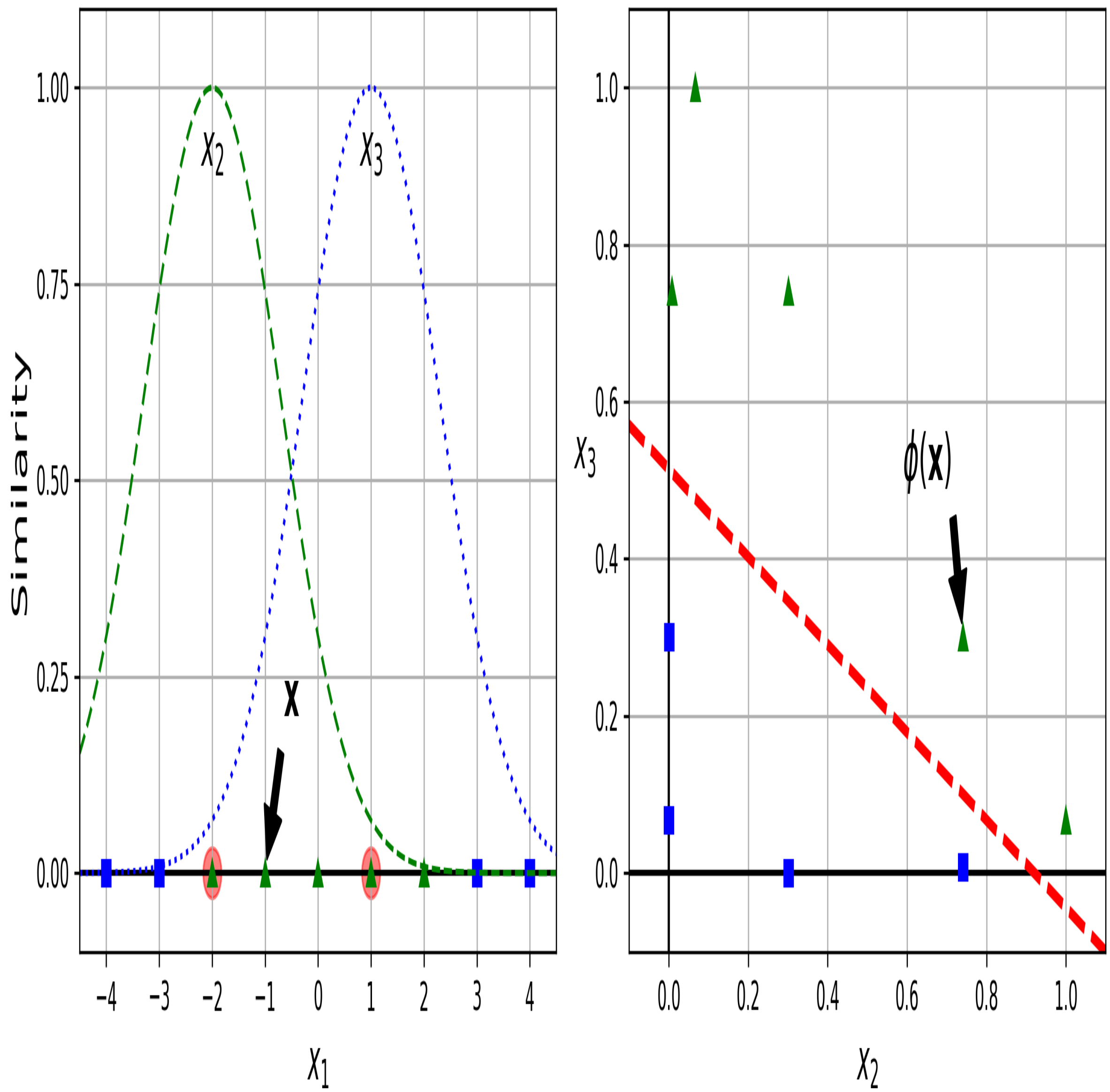


Figure 5-8. Similarity features using the Gaussian RBF

You may wonder how to select the landmarks. The simplest approach is to create a landmark at the location of each and every instance in the dataset. Doing that creates many dimensions and thus increases the chances that the transformed training set will be linearly separable. The downside is that a training set with *m* instances and *n* features gets transformed into a training set with *m* instances and *m* features (assuming you drop the original features). If your training set is very large, you end up with an equally large number of features.

Gaussian RBF Kernel

Just like the polynomial features method, the similarity features method can be useful with any Machine Learning algorithm, but it may be computationally expensive to compute all the additional features, especially on large training sets. Once again the kernel trick does its SVM magic, making it possible to obtain a similar result as if you had added many similarity features, but without actually doing so. Let's try the `SVC` class with the Gaussian RBF kernel:

```
rbf_kernel_svm_clf = make_pipeline(StandardScaler(),
                                   SVC(kernel="rbf", gamma=5, C=0.001))
rbf_kernel_svm_clf.fit(X, y)
```

This model is represented at the bottom left in Figure 5-9. The other plots show models trained with different values of hyperparameters `gamma` (γ) and `C`. Increasing `gamma` makes the bell-shaped curve narrower (see the lefthand plots in Figure 5-8). As a result, each instance's range of influence is smaller: the decision boundary ends up being more irregular, wiggling around individual instances. Conversely, a small `gamma` value makes the bell-shaped curve wider: instances have a larger range of influence, and the decision boundary ends up smoother. So γ acts like a regularization hyperparameter: if your model is overfitting, you should reduce γ; if it is underfitting, you should increase γ (similar to the `C` hyperparameter).

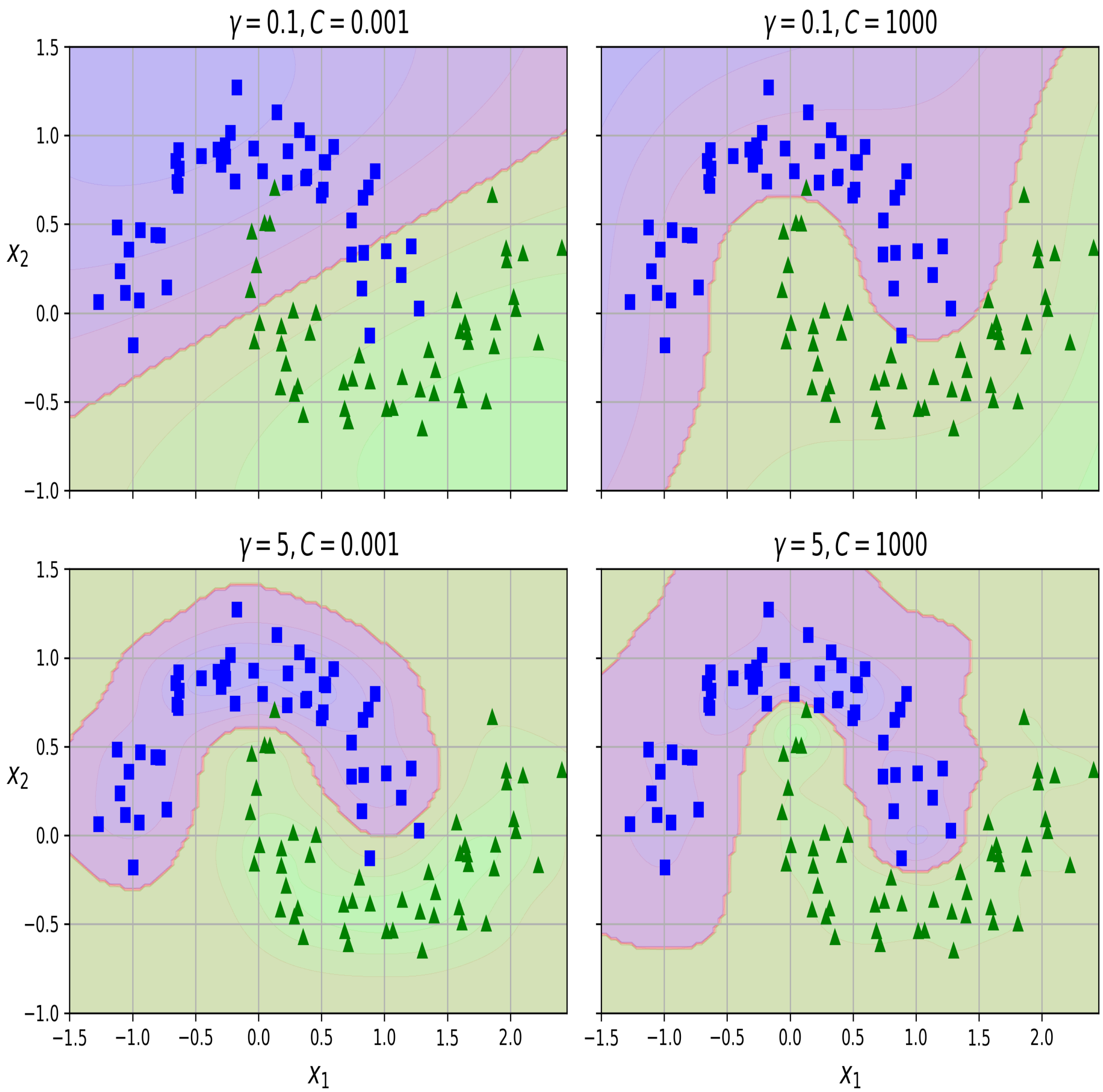


Figure 5-9. SVM classifiers using an RBF kernel

Other kernels exist but are used much more rarely. Some kernels are specialized for specific data structures. *String kernels* are sometimes used when classifying text documents or DNA sequences (e.g., using the *string subsequence kernel* or kernels based on the *Levenshtein distance*).

> **TIP**
>
> With so many kernels to choose from, how can you decide which one to use? As a rule of thumb, you should always try the linear kernel first. The `LinearSVC` class is much faster than `SVC(kernel="linear")`, especially if the training set is very large. If it is not too large, you should also try kernelized SVMs, starting with the Gaussian RBF kernel; it often works really well. Then if you have spare time and computing power, you can experiment with a few other kernels, using hyperparameter search. If there are kernels specialized for your training set's data structure, make sure to give them a try too.

SVM Classes and Computational Complexity

The `LinearSVC` class is based on the `liblinear` library, which implements an optimized algorithm for linear SVMs.[1] It does not support the kernel trick, but it scales almost linearly with the number of training instances and the number of features. Its training time complexity is roughly $O(m \times n)$. The algorithm takes longer if you require very high precision. This is controlled by the tolerance hyperparameter ϵ (called `tol` in Scikit-Learn). In most classification tasks, the default tolerance is fine.

The `SVC` class is based on the `libsvm` library, which implements an algorithm that supports the kernel trick.[2] The training time complexity is usually between $O(m^2 \times n)$ and $O(m^3 \times n)$. Unfortunately, this means that it gets dreadfully slow when the number of training instances gets large (e.g., hundreds of thousands of instances). This algorithm is best for small or medium-sized nonlinear training sets. It scales well with the number of features, especially with *sparse features* (i.e., when each instance has few nonzero features). In this case, the algorithm scales roughly with the average number of nonzero features per instance. Table 5-1 compares Scikit-Learn's SVM classification classes.

Lastly, the `SGDClassifier` class also performs large-margin classification by default, and its hyperparameters can be adjusted to produce similar results as the linear SVMs, especially the regularization hyperparameters (`alpha` and `penalty`) and the `learning_rate`. For training, it uses Stochastic Gradient Descent (see Chapter 4), which allows incremental learning and uses little memory. Moreover, it scales very well, as its computational complexity is $O(m \times n)$.

Table 5-1. Comparison of Scikit-Learn classes for SVM class

i
f
i
c
a
t
i
o
n

Class	Time Complexity	Out-of-core support	Scaling required	Kernel trick
`LinearSVC`	$O(m \times n)$	No	Yes	No
`SVC`	$O(m^2 \times n)$ to $O(m^3 \times n)$	No	Yes	Yes
`SGDClassifier`	$O(m \times n)$	Yes	Yes	No

Now let's see how the SVM algorithm can also be used for linear and nonlinear regression.

SVM Regression

To use SVMs for regression instead of classification, the trick is to tweak the objective: instead of trying to fit the largest possible street between two classes while limiting margin violations, SVM Regression tries to fit as many instances as possible *on* the street while limiting margin violations (i.e., instances *off* the street). The width of the street is controlled by a hyperparameter, ϵ. Figure 5-10 shows two linear SVM Regression models trained on some linear data, one with a small margin ($\epsilon = 0.5$) and the other with a large margin ($\epsilon = 1.5$).

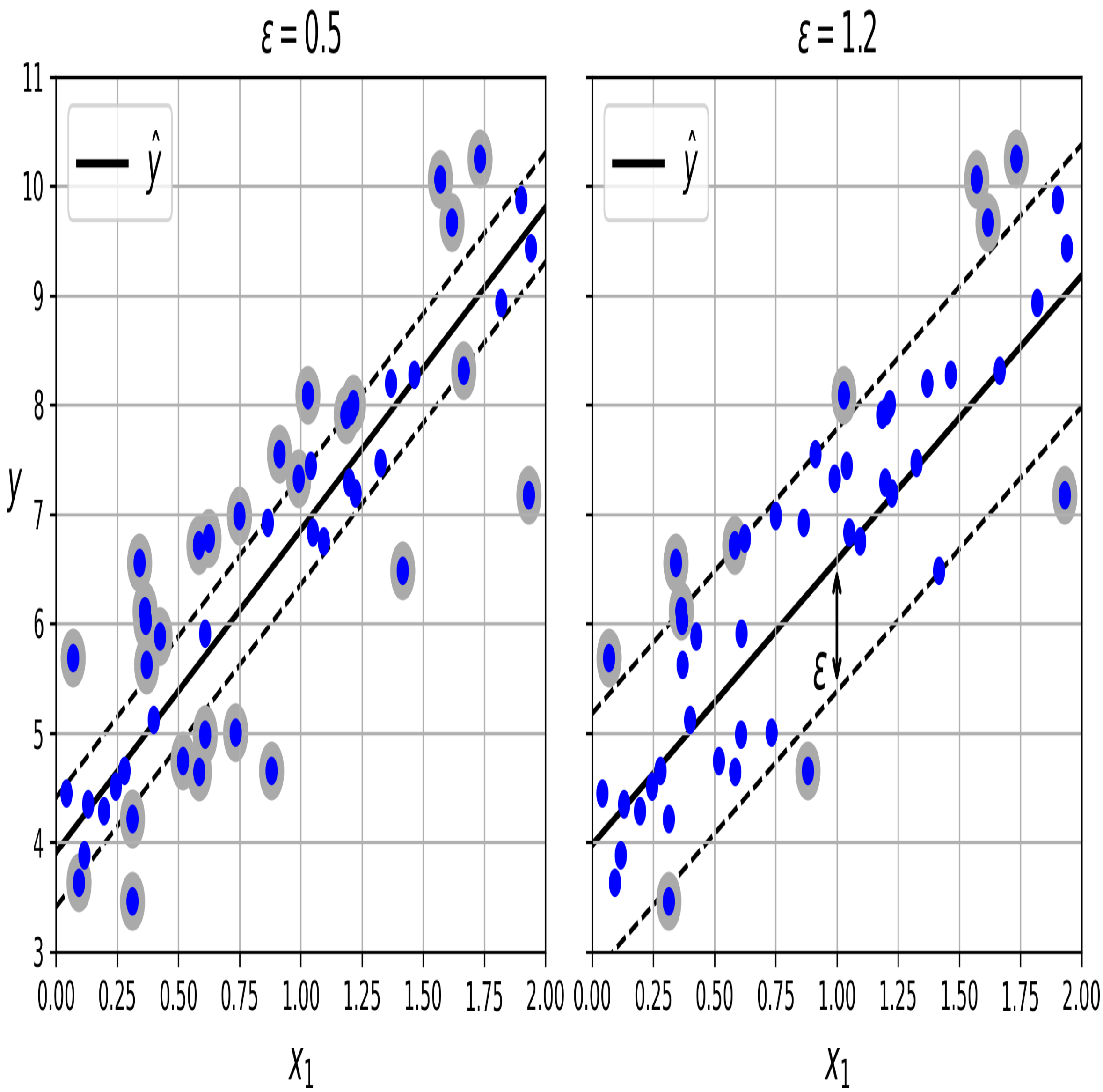


Figure 5-10. SVM Regression

Reducing ϵ increases the number of support vectors, which regularizes the model. Moreover, if you add more training instances within the margin, it will not affect the model's predictions; thus, the model is said to be *ϵ-insensitive*.

You can use Scikit-Learn's `LinearSVR` class to perform linear SVM Regression. The following code produces the model represented on the left in Figure 5-10:

```
from sklearn.svm import LinearSVR

X, y = [...]  # a linear dataset
svm_reg = make_pipeline(StandardScaler(),
                        LinearSVR(epsilon=0.5, random_state=42))
svm_reg.fit(X, y)
```

To tackle nonlinear regression tasks, you can use a kernelized SVM model. Figure 5-11 shows SVM Regression on a random quadratic training set, using a second-degree polynomial kernel. There is some regularization in the left plot (i.e., a small `C` value), and much less in the right plot (i.e., a large `C` value).

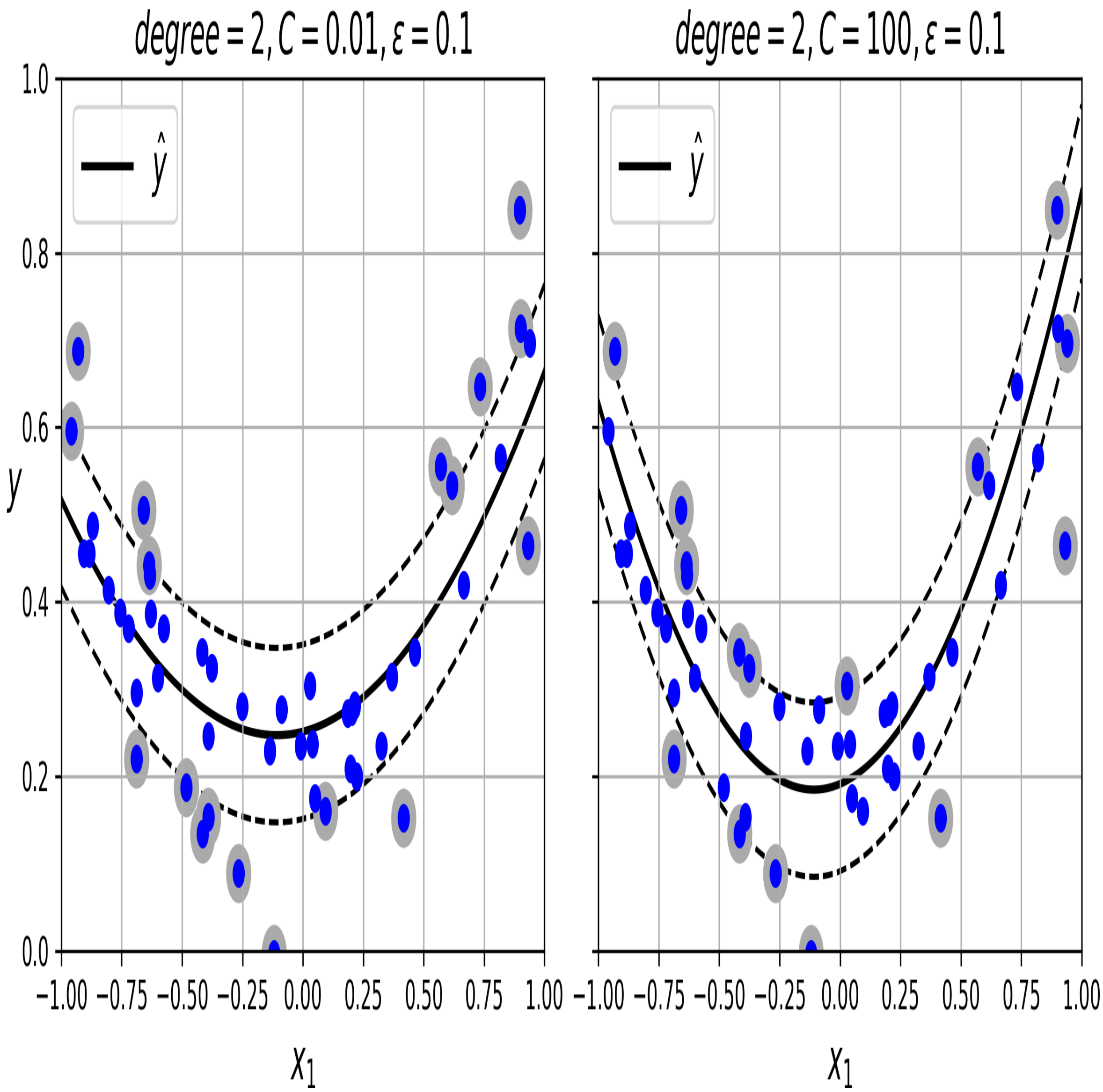


Figure 5-11. SVM Regression using a second-degree polynomial kernel

The following code uses Scikit-Learn's `SVR` class (which supports the kernel trick) to produce the model represented on the left in Figure 5-11:

```
from sklearn.svm import SVR

X, y = [...]  # a quadratic dataset
svm_poly_reg = make_pipeline(StandardScaler(),
                             SVR(kernel="poly", degree=2, C=0.01, epsilon=0.1))
svm_poly_reg.fit(X, y)
```

The `SVR` class is the regression equivalent of the `SVC` class, and the `LinearSVR` class is the regression equivalent of the `LinearSVC` class. The `LinearSVR` class scales linearly with the size of the training set (just like the `LinearSVC` class), while the `SVR` class gets much too slow when the training set grows very large (just like the `SVC` class).

NOTE

SVMs can also be used for novelty detection, as we will see in Chapter 9.

The rest of this chapter explains how SVMs make predictions and how their training algorithms work, starting with linear SVM classifiers. If you are just getting started with Machine Learning, you can safely skip this and go straight to the exercises at the end of this chapter, and come back later when you want to get a deeper understanding of SVMs.

Under The Hood of Linear SVM Classifiers

The linear SVM classifier model predicts the class of a new instance **x** by first computing the decision function $\boldsymbol{\theta}^\intercal \mathbf{x} = \theta_0 x_0 + \cdots + \theta_n x_n$, where x_0 is the bias feature (always equal to 1). If the result is positive, then the predicted class $\hat{y}$ is the positive class (1), otherwise it is the negative class (0). This is exactly like `LogisticRegression` (discussed in Chapter 4).

NOTE

Up to now, I have used the convention of putting all the model parameters in one vector $\boldsymbol{\theta}$, including the bias term $\boldsymbol{\theta}_0$ and the input feature weights $\boldsymbol{\theta}_1$ to $\boldsymbol{\theta}_n$. This required adding a bias input $x_0 = 1$ to all instances. Another very common convention is to separate the bias term b (equal to $\boldsymbol{\theta}_0$), and the feature weights vector **w** (containing $\boldsymbol{\theta}_1$ to $\boldsymbol{\theta}_n$). In this case, no bias feature needs to be added to the input feature vectors, and the linear SVM's decision function is equal to $\mathbf{w}^\intercal \mathbf{x} + b = w_1 x_1 + \cdots + w_n x_n + b$. I will use this convention throughout the rest of this book.

So making predictions with a linear SVM classifier is quite straightforward. How about training? Well, it requires finding the weights vector **w** and the bias term b that make the "street" (i.e., the margin) as wide as possible while limiting the number of margin violations. Let's start with the width of the street: to make it larger, we need to make **w** smaller. This may be easier to visualize in 2D, as shown in Figure 5-12. Let's define the borders of the street as the points where the decision function is equal to –1 or +1. On the left plot, the weight w_1 is 1, so the points at which $w_1 x_1 = –1$ or $+1$ are $x_1 = –1$ and $+1$: therefore the margin's size is 2. On the right plot, the weight is 0.5, so the points at which $w_1 x_1 = –1$ or $+1$ are $x_1 = –2$ and $+2$: the margin's size is 4. So we need to keep **w** as small as possible. Note that the bias term b has no influence on the size of the margin: tweaking it just shifts the margin around, without affecting its size.

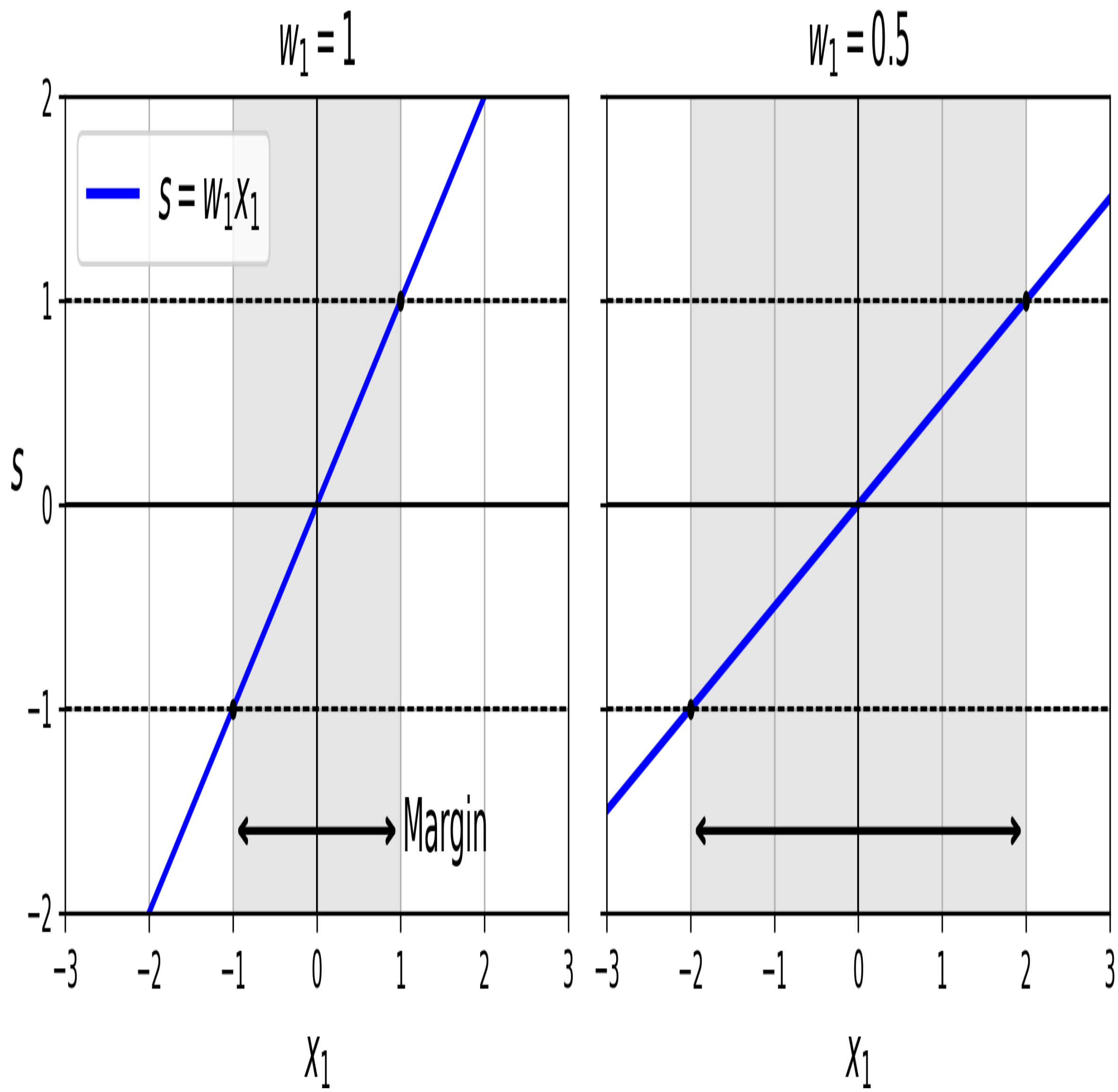


Figure 5-12. A smaller weight vector results in a larger margin

We also want to avoid margin violations, so we need the decision function to be greater than 1 for all positive training instances and lower than –1 for negative training instances. If we define $t^{(i)} = -1$ for negative instances (when $y^{(i)} = 0$) and $t^{(i)} = 1$ for positive instances (when $y^{(i)} = 1$), then we can write this constraint as $t^{(i)}(\mathbf{w}^\top \mathbf{x}^{(i)} + b) \geq 1$ for all instances.

We can therefore express the hard margin linear SVM classifier objective as the constrained optimization problem in Equation 5-1.

Equation 5-1. Hard margin linear SVM classifier objective

$$\begin{aligned} &\underset{\mathbf{w},b}{\text{minimize}} && \frac{1}{2}\mathbf{w}^\top\mathbf{w} \\ &\text{subject to} && t^{(i)}\left(\mathbf{w}^\top\mathbf{x}^{(i)} + b\right) \geq 1 \quad \text{for } i = 1, 2, \cdots, m \end{aligned}$$

NOTE

We are minimizing ½ $\mathbf{w}^\intercal \mathbf{w}$, which is equal to ½$\| \mathbf{w} \|^2$, rather than minimizing $\| \mathbf{w} \|$ (the norm of **w**). Indeed, ½$\| \mathbf{w} \|^2$ has a nice, simple derivative (it is just **w**), while $\| \mathbf{w} \|$ is not differentiable at **w** = 0. Optimization algorithms often work much better on differentiable functions.

To get the soft margin objective, we need to introduce a *slack variable* $\zeta^{(i)} \geq 0$ for each instance:[3] $\zeta^{(i)}$ measures how much the i^{th} instance is allowed to violate the margin. We now have two conflicting objectives: make the slack variables as small as possible to reduce the margin violations, and make ½ $\mathbf{w}^\intercal \mathbf{w}$ as small as possible to increase the margin. This is where the `C` hyperparameter comes in: it allows us to define the tradeoff between these two objectives. This gives us the constrained optimization problem in Equation 5-2.

Equation 5-2. Soft margin linear SVM classifier objective

$$\begin{aligned} &\underset{\mathbf{w},b,\zeta}{\text{minimize}} \quad \frac{1}{2}\mathbf{w}^\intercal \mathbf{w} + C\sum_{i=1}^{m}\zeta^{(i)} \\ &\text{subject to} \quad t^{(i)}\left(\mathbf{w}^\intercal \mathbf{x}^{(i)} + b\right) \geq 1 - \zeta^{(i)} \quad \text{and} \quad \zeta^{(i)} \geq 0 \quad \text{for } i = 1, 2, \cdots, m \end{aligned}$$

The hard margin and soft margin problems are both convex quadratic optimization problems with linear constraints. Such problems are known as *Quadratic Programming* (QP) problems. Many off-the-shelf solvers are available to solve QP problems by using a variety of techniques that are outside the scope of this book.[4]

So using a QP solver is one way to train an SVM. Another is to use Gradient Descent to minimize the *Hinge loss* or the *squared Hinge loss* (see Figure 5-13). Given an instance **x** of the positive class (i.e., with $t = 1$), the loss is zero if the output s of the decision function ($s = \mathbf{w}^\intercal \mathbf{x} + b$) is greater or equal to 1. This happens when the instance is off the street and on the positive side. Given an instance of the negative class (i.e., with $t = -1$), the loss is zero if $s \leq -1$. This happens when the instance is off the street and on the negative side. The further away an instance is from the correct side of the margin, the higher the loss: it grows linearly for the Hinge loss, and quadratically for the squared Hinge loss. This makes the squared Hinge loss more sensitive to outliers. However, if the dataset is clean, it tends to converge faster. By default, `LinearSVC` uses the squared Hinge loss, while `SGDClassifier` uses the Hinge loss. Both classes let you choose the loss by setting the `loss` hyperparameter to `"hinge"` or `"squared_hinge"`. The `SVC` class's optimization algorithm finds a similar solution as minimizing the Hinge loss.

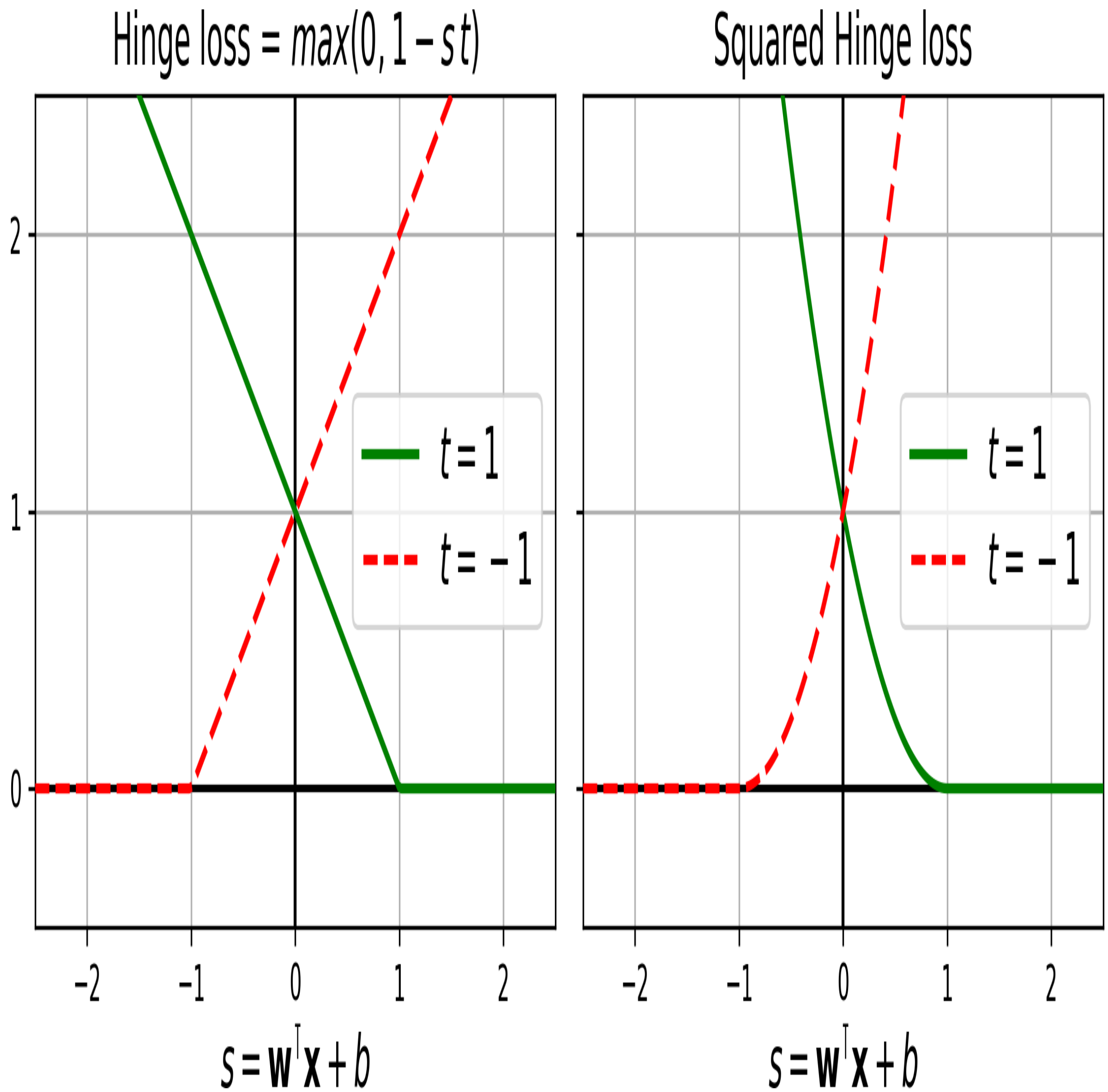


Figure 5-13. The Hinge loss (left) and the Squared Hinge loss (right)

There's yet another way to train a linear SVM classifier: solving the dual problem.

The Dual Problem

Given a constrained optimization problem, known as the *primal problem*, it is possible to express a different but closely related problem, called its *dual problem*. The solution to the dual problem typically gives a lower bound to the solution of the primal problem, but under some conditions it can have the same solution as the primal problem. Luckily, the SVM problem happens to meet these conditions,[5] so you can choose to solve the primal problem or the dual problem; both will have the same solution. Equation 5-3 shows the dual form of the linear SVM objective. If you are interested in knowing how to derive the dual problem from the primal problem, see the extra material section in the notebook.

Equation 5-3. Dual form of the linear SVM objective

$$\underset{\boldsymbol{\alpha}}{\text{minimize}} \ \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m}\alpha^{(i)}\alpha^{(j)}t^{(i)}t^{(j)}\mathbf{x}^{(i)\intercal}\mathbf{x}^{(j)} \quad - \quad \sum_{i=1}^{m}\alpha^{(i)}\text{subject to } \alpha^{(i)} \geq 0 \text{ for all } i = 1, 2, \ldots, m \text{ and } \sum_{i=1}^{m}\alpha^{(}$$

Once you find the vector $\widehat{\boldsymbol{\alpha}}$ that minimizes this equation (using a QP solver), use Equation 5-4 to compute $\widehat{\mathbf{w}}$ and $\hat{b}$ that minimize the primal problem.

Equation 5-4. From the dual solution to the primal solution

$$\widehat{\mathbf{w}} = \sum_{i=1}^{m}\widehat{\alpha}^{(i)}t^{(i)}\mathbf{x}^{(i)}$$

$$\hat{b} = \frac{1}{n_s}\sum_{\substack{i=1 \\ \widehat{\alpha}^{(i)}>0}}^{m}\left(t^{(i)} - \widehat{\mathbf{w}}^\intercal\mathbf{x}^{(i)}\right)$$

Where n_s is the number of support vectors.

The dual problem is faster to solve than the primal one when the number of training instances is smaller than the number of features. More importantly, the dual problem makes the kernel trick possible, while the primal does not. So what is this kernel trick, anyway?

Kernelized SVMs

Suppose you want to apply a second-degree polynomial transformation to a two-dimensional training set (such as the moons training set), then train a linear SVM classifier on the transformed training set. Equation 5-5 shows the second-degree polynomial mapping function ϕ that you want to apply.

Equation 5-5. Second-degree polynomial mapping

$$\phi(\mathbf{x}) = \phi\left(\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}\right) = \begin{pmatrix} {x_1}^2 \\ \sqrt{2}\,x_1x_2 \\ {x_2}^2 \end{pmatrix}$$

Notice that the transformed vector is 3D instead of 2D. Now let's look at what happens to a couple of 2D vectors, **a** and **b**, if we apply this second-degree polynomial mapping and then compute the dot product[6] of the transformed vectors (See Equation 5-6).

Equation 5-6. Kernel trick for a second-degree polynomial mapping

$$\begin{aligned}
\phi(\mathbf{a})^\intercal\phi\left(\mathbf{b}\right) \quad &= \begin{pmatrix} {a_1}^2 \\ \sqrt{2}\,a_1a_2 \\ {a_2}^2 \end{pmatrix}^\intercal \begin{pmatrix} {b_1}^2 \\ \sqrt{2}\,b_1b_2 \\ {b_2}^2 \end{pmatrix} = {a_1}^2{b_1}^2 + 2a_1b_1a_2b_2 + {a_2}^2{b_2}^2 \\
&= \left(a_1b_1 + a_2b_2\right)^2 = \left(\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}^\intercal\begin{pmatrix} b_1 \\ b_2 \end{pmatrix}\right)^2 = \left(\mathbf{a}^\intercal\mathbf{b}\right)^2
\end{aligned}$$

How about that? The dot product of the transformed vectors is equal to the square of the dot product of the original vectors: $\phi(\mathbf{a})^\intercal\,\phi(\mathbf{b}) = (\mathbf{a}^\intercal\,\mathbf{b})^2$.

Here is the key insight: if you apply the transformation ϕ to all training instances, then the dual problem (see Equation 5-3) will contain the dot product $\phi(\mathbf{x}^{(i)})^\intercal\,\phi(\mathbf{x}^{(j)})$. But if ϕ is the second-degree polynomial transformation defined in Equation 5-5, then you can replace this dot product of transformed vectors simply by $\left(\mathbf{x}^{(i)\intercal}\mathbf{x}^{(j)}\right)^2$. So, you don't need to transform the training instances at all; just replace the dot product by its square in Equation 5-3. The result will be strictly the same as if you had gone through the trouble of transforming the training set then fitting a linear SVM algorithm, but this trick makes the whole process much more computationally efficient.

The function $K(\mathbf{a}, \mathbf{b}) = (\mathbf{a}^\intercal \mathbf{b})^2$ is a second-degree polynomial kernel. In Machine Learning, a *kernel* is a function capable of computing the dot product $\phi(\mathbf{a})^\intercal \phi(\mathbf{b})$, based only on the original vectors **a** and **b**, without having to compute (or even to know about) the transformation ϕ. Equation 5-7 lists some of the most commonly used kernels.

Equation 5-7. Common kernels

$$\begin{aligned} \text{Linear:} \quad & K(\mathbf{a}, \mathbf{b}) = \mathbf{a}^\intercal \mathbf{b} \\ \text{Polynomial:} \quad & K(\mathbf{a}, \mathbf{b}) = \left(\gamma \mathbf{a}^\intercal \mathbf{b} + r\right)^d \\ \text{Gaussian RBF:} \quad & K(\mathbf{a}, \mathbf{b}) = \exp\left(-\gamma \|\mathbf{a} - \mathbf{b}\|^2\right) \\ \text{Sigmoid:} \quad & K(\mathbf{a}, \mathbf{b}) = \tanh\left(\gamma \mathbf{a}^\intercal \mathbf{b} + r\right) \end{aligned}$$

MERCER'S THEOREM

According to *Mercer's theorem*, if a function $K(\mathbf{a}, \mathbf{b})$ respects a few mathematical conditions called *Mercer's conditions* (e.g., K must be continuous and symmetric in its arguments so that $K(\mathbf{a}, \mathbf{b}) = K(\mathbf{b}, \mathbf{a})$, etc.), then there exists a function ϕ that maps **a** and **b** into another space (possibly with much higher dimensions) such that $K(\mathbf{a}, \mathbf{b}) = \phi(\mathbf{a})^\intercal \phi(\mathbf{b})$. You can use K as a kernel because you know ϕ exists, even if you don't know what ϕ is. In the case of the Gaussian RBF kernel, it can be shown that ϕ maps each training instance to an infinite-dimensional space, so it's a good thing you don't need to actually perform the mapping!

Note that some frequently used kernels (such as the sigmoid kernel) don't respect all of Mercer's conditions, yet they generally work well in practice.

There is still one loose end we must tie up. Equation 5-4 shows how to go from the dual solution to the primal solution in the case of a linear SVM classifier. But if you apply the kernel trick, you end up with equations that include $\phi(x^{(i)})$. In fact, $\hat{\mathbf{w}}$ must have the same number of dimensions as $\phi(x^{(i)})$, which may be huge or even infinite, so you can't compute it. But how can you make predictions without knowing $\hat{\mathbf{w}}$? Well, the good news is that you can plug the formula for $\hat{\mathbf{w}}$ from Equation 5-4 into the decision function for a new instance $\mathbf{x}^{(n)}$, and you get an equation with only dot products between input vectors. This makes it possible to use the kernel trick (Equation 5-8).

Equation 5-8. Making predictions with a kernelized SVM

$$\begin{aligned} h_{\hat{\mathbf{w}}, \hat{b}}\left(\phi\left(\mathbf{x}^{(n)}\right)\right) &= \hat{\mathbf{w}}^\intercal \phi\left(\mathbf{x}^{(n)}\right) + \hat{b} = \left(\sum_{i=1}^{m} \hat{\alpha}^{(i)} t^{(i)} \phi\left(\mathbf{x}^{(i)}\right)\right)^\intercal \phi\left(\mathbf{x}^{(n)}\right) + \hat{b} \\ &= \sum_{i=1}^{m} \hat{\alpha}^{(i)} t^{(i)} \left(\phi\left(\mathbf{x}^{(i)}\right)^\intercal \phi\left(\mathbf{x}^{(n)}\right)\right) + \hat{b} \\ &= \sum_{\substack{i=1 \\ \hat{\alpha}^{(i)} > 0}}^{m} \hat{\alpha}^{(i)} t^{(i)} K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(n)}\right) + \hat{b} \end{aligned}$$

Note that since $\alpha^{(i)} \neq 0$ only for support vectors, making predictions involves computing the dot product of the new input vector $\mathbf{x}^{(n)}$ with only the support vectors, not all the training instances. Of course, you need to use the same trick to compute the bias term $\hat{b}$ (Equation 5-9).

Equation 5-9. Using the kernel trick to compute the bias term

$$\begin{aligned}\hat{b} &= \frac{1}{n_s}\sum_{\substack{i=1\\ \hat{\alpha}^{(i)}>0}}^{m}\left(t^{(i)} - \hat{\mathbf{w}}^\intercal \phi\left(\mathbf{x}^{(i)}\right)\right) = \frac{1}{n_s}\sum_{\substack{i=1\\ \hat{\alpha}^{(i)}>0}}^{m}\left(t^{(i)} - \left(\sum_{j=1}^{m}\hat{\alpha}^{(j)} t^{(j)} \phi\left(\mathbf{x}^{(j)}\right)\right)^\intercal \phi\left(\mathbf{x}^{(i)}\right)\right)\\ &= \frac{1}{n_s}\sum_{\substack{i=1\\ \hat{\alpha}^{(i)}>0}}^{m}\left(t^{(i)} - \sum_{\substack{j=1\\ \hat{\alpha}^{(j)}>0}}^{m}\hat{\alpha}^{(j)} t^{(j)} K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right)\right)\end{aligned}$$

If you are starting to get a headache, it's perfectly normal: it's an unfortunate side effect of the kernel trick.

> **NOTE**
>
> It is also possible to implement online kernelized SVMs, capable of incremental learning, as described in the papers "Incremental and Decremental Support Vector Machine Learning"[7] and "Fast Kernel Classifiers with Online and Active Learning".[8] These kernelized SVMs are implemented in Matlab and C++. But for large-scale nonlinear problems, you may want to consider using Random Forests (see Chapter 7) or neural networks (see Part II).

Exercises

1. What is the fundamental idea behind Support Vector Machines?
2. What is a support vector?
3. Why is it important to scale the inputs when using SVMs?
4. Can an SVM classifier output a confidence score when it classifies an instance? What about a probability?
5. How can you choose between `LinearSVC`, `SVC`, or `SGDClassifier`?
6. Say you've trained an SVM classifier with an RBF kernel, but it seems to underfit the training set. Should you increase or decrease γ (`gamma`)? What about `C`?
7. What does it mean for a model to be *ϵ-insensitive*?
8. What is the point of using the kernel trick?
9. Train a `LinearSVC` on a linearly separable dataset. Then train an `SVC` and a `SGDClassifier` on the same dataset. See if you can get them to produce roughly the same model.
10. Train an SVM classifier on the Wine dataset, which you can load using `sklearn.datasets.load_wine()`. This dataset contains the chemical analysis of 178 wine samples produced by 3 different cultivators: the goal is to train a classification model capable of predicting the cultivator based on the wine's chemical analysis. Since SVM classifiers are binary classifiers, you will need to use one-versus-all to classify all 3 classes. What accuracy can you reach?
11. Train and fine-tune an SVM regressor on the California housing dataset. You can use the original dataset rather than the tweaked version we used in Chapter 2. The original dataset can be fetched using `sklearn.datasets.fetch_california_housing()`. The targets represent hundreds of thousands of dollars. Since there are over 20,000 instances, SVMs can be slow, so for hyperparameter tuning you should use much less instances (e.g., 2,000), to test many more hyperparameter combinations. What is your best model's RMSE?

Solutions to these exercises are available at the end of this chapter's notebook, at *https://homl.info/colab3*.

---

1 Chih-Jen Lin et al., "A Dual Coordinate Descent Method for Large-Scale Linear SVM," *Proceedings of the 25th International Conference on Machine Learning* (2008): 408–415.

2 John Platt, “Sequential Minimal Optimization: A Fast Algorithm for Training Support Vector Machines” (Microsoft Research technical report, April 21, 1998), *https://www.microsoft.com/en-us/research/wp-content/uploads/2016/02/tr-98-14.pdf*.

3 Zeta (ζ) is the sixth letter of the Greek alphabet.

4 To learn more about Quadratic Programming, you can start by reading Stephen Boyd and Lieven Vandenberghe’s book *Convex Optimization* (Cambridge University Press, 2004) or watch Richard Brown’s series of video lectures.

5 The objective function is convex, and the inequality constraints are continuously differentiable and convex functions.

6 As explained in Chapter 4, the dot product of two vectors **a** and **b** is normally noted $\mathbf{a} \cdot \mathbf{b}$. However, in Machine Learning, vectors are frequently represented as column vectors (i.e., single-column matrices), so the dot product is achieved by computing $\mathbf{a}^\intercal\mathbf{b}$. To remain consistent with the rest of the book, we will use this notation here, ignoring the fact that this technically results in a single-cell matrix rather than a scalar value.

7 Gert Cauwenberghs and Tomaso Poggio, “Incremental and Decremental Support Vector Machine Learning,” *Proceedings of the 13th International Conference on Neural Information Processing Systems* (2000): 388–394.

8 Antoine Bordes et al., “Fast Kernel Classifiers with Online and Active Learning,” *Journal of Machine Learning Research* 6 (2005): 1579–1619.

Chapter 6. Decision Trees

A NOTE FOR EARLY RELEASE READERS

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.

This will be the 6th chapter of the final book. Notebooks are available on GitHub at *https://github.com/ageron/handson-ml3*. Datasets are available at *https://github.com/ageron/data*.

If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the editoor at ntache@oreilly.com.

Decision Trees are versatile Machine Learning algorithms that can perform both classification and regression tasks, and even multioutput tasks. They are powerful algorithms, capable of fitting complex datasets. For example, in Chapter 2 you trained a `DecisionTreeRegressor` model on the California housing dataset, fitting it perfectly (actually, overfitting it).

Decision Trees are also the fundamental components of Random Forests (see Chapter 7), which are among the most powerful Machine Learning algorithms available today.

In this chapter we will start by discussing how to train, visualize, and make predictions with Decision Trees. Then we will go through the CART training algorithm used by Scikit-Learn, and we will discuss how to regularize trees and use them for regression tasks. Finally, we will discuss some of the limitations of Decision Trees.

Training and Visualizing a Decision Tree

To understand Decision Trees, let's build one and take a look at how it makes predictions. The following code trains a `DecisionTreeClassifier` on the iris dataset (see Chapter 4):

```
from sklearn.datasets import load_iris
from sklearn.tree import DecisionTreeClassifier
```

```python
iris = load_iris(as_frame=True)
X_iris = iris.data[["petal length (cm)", "petal width (cm)"]].values
y_iris = iris.target

tree_clf = DecisionTreeClassifier(max_depth=2, random_state=42)
tree_clf.fit(X_iris, y_iris)
```

You can visualize the trained Decision Tree by first using the `export_graphviz()` method to output a graph definition file called *iris_tree.dot*:

```python
from sklearn.tree import export_graphviz

export_graphviz(
        tree_clf,
        out_file="iris_tree.dot",
        feature_names=["petal length (cm)", "petal width (cm)"],
        class_names=iris.target_names,
        rounded=True,
        filled=True
    )
```

Then you can use `graphviz.Source.from_file()` to load and display the file in a Jupyter notebook:

```python
from graphviz import Source

Source.from_file("iris_tree.dot")
```

Graphviz is an open source graph visualization software package. It also includes a `dot` command-line tool to convert *.dot* files to a variety of formats, such as PDF or PNG.

Your first Decision Tree looks like Figure 6-1.

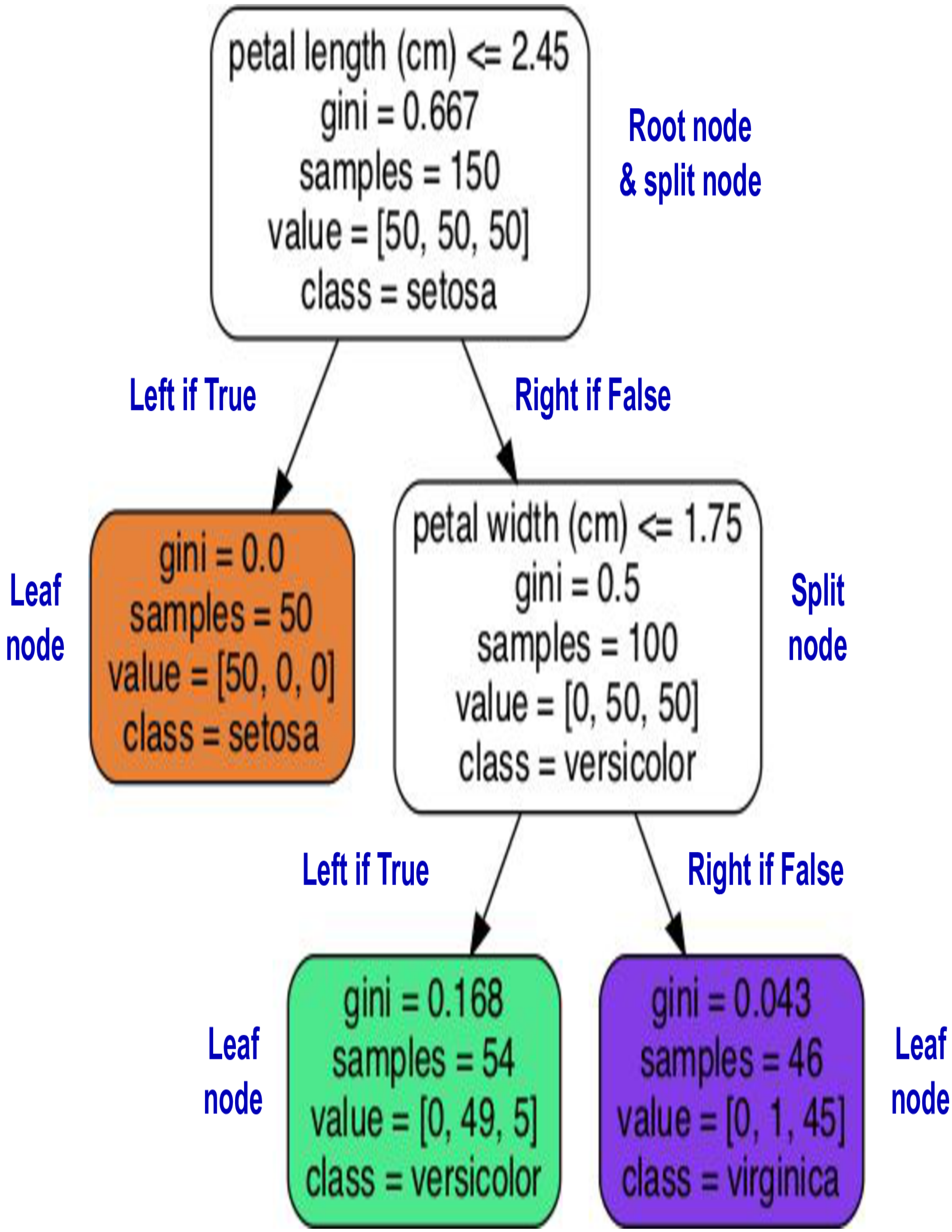


Figure 6-1. Iris Decision Tree

Making Predictions

Let’s see how the tree represented in Figure 6-1 makes predictions. Suppose you find an iris plant and you want to classify it based on its petals. You start at the *root node* (depth 0, at the top): this node asks whether the flower’s petal length is smaller than 2.45 cm. If it is, then you move down to the root’s left child node (depth 1, left). In this case, it is a *leaf node* (i.e., it does not have any child nodes), so it does not ask any questions: simply look at the predicted class for that node, and the Decision Tree predicts that your flower is an *Iris setosa* (`class=setosa`).

Now suppose you find another flower, and this time the petal length is greater than 2.45 cm. You must move down to the root’s right child node (depth 1, right), which is not a leaf node, it’s a *split node*, so it asks another question: is the petal width smaller than 1.75 cm? If it is, then your flower is most likely an *Iris versicolor* (depth 2, left). If not, it is likely an *Iris virginica* (depth 2, right). It’s really that simple.

> **NOTE**
>
> One of the many qualities of Decision Trees is that they require very little data preparation. In fact, they don’t require feature scaling or centering at all.

A node’s `samples` attribute counts how many training instances it applies to. For example, 100 training instances have a petal length greater than 2.45 cm (depth 1, right), and of those 100, 54 have a petal width smaller than 1.75 cm (depth 2, left). A node’s `value` attribute tells you how many training instances of each class this node applies to: for example, the bottom-right node applies to 0 *Iris setosa*, 1 *Iris versicolor*, and 45 *Iris virginica*. Finally, a node’s `gini` attribute measures its *Gini impurity*: a node is “pure” (`gini=0`) if all training instances it applies to belong to the same class. For example, since the depth-1 left node applies only to *Iris setosa* training instances, it is pure and its Gini impurity is 0. Equation 6-1 shows how the training algorithm computes the Gini impurity G_i of the i^{th} node. The depth-2 left node has a Gini impurity equal to $1 – (0/54)^2 – (49/54)^2 – (5/54)^2 \approx 0.168$.

Equation 6-1. Gini impurity

$$G_i = 1 - \sum_{k=1}^{n} {p_{i,k}}^2$$

In this equation:

- G_i is the Gini impurity of the i^{th} node.

- $p_{i,k}$ is the ratio of class k instances among the training instances in the i^{th} node.

> **NOTE**
>
> Scikit-Learn uses the CART algorithm, which produces only *binary trees*, meaning trees where split nodes always have exactly two children (i.e., questions only have yes/no answers). However, other algorithms such as ID3 can produce Decision Trees with nodes that have more than two children.

Figure 6-2 shows this Decision Tree's decision boundaries. The thick vertical line represents the decision boundary of the root node (depth 0): petal length = 2.45 cm. Since the lefthand area is pure (only *Iris setosa*), it cannot be split any further. However, the righthand area is impure, so the depth-1 right node splits it at petal width = 1.75 cm (represented by the dashed line). Since `max_depth` was set to 2, the Decision Tree stops right there. If you set `max_depth` to 3, then the two depth-2 nodes would each add another decision boundary (represented by the two vertical dotted lines).

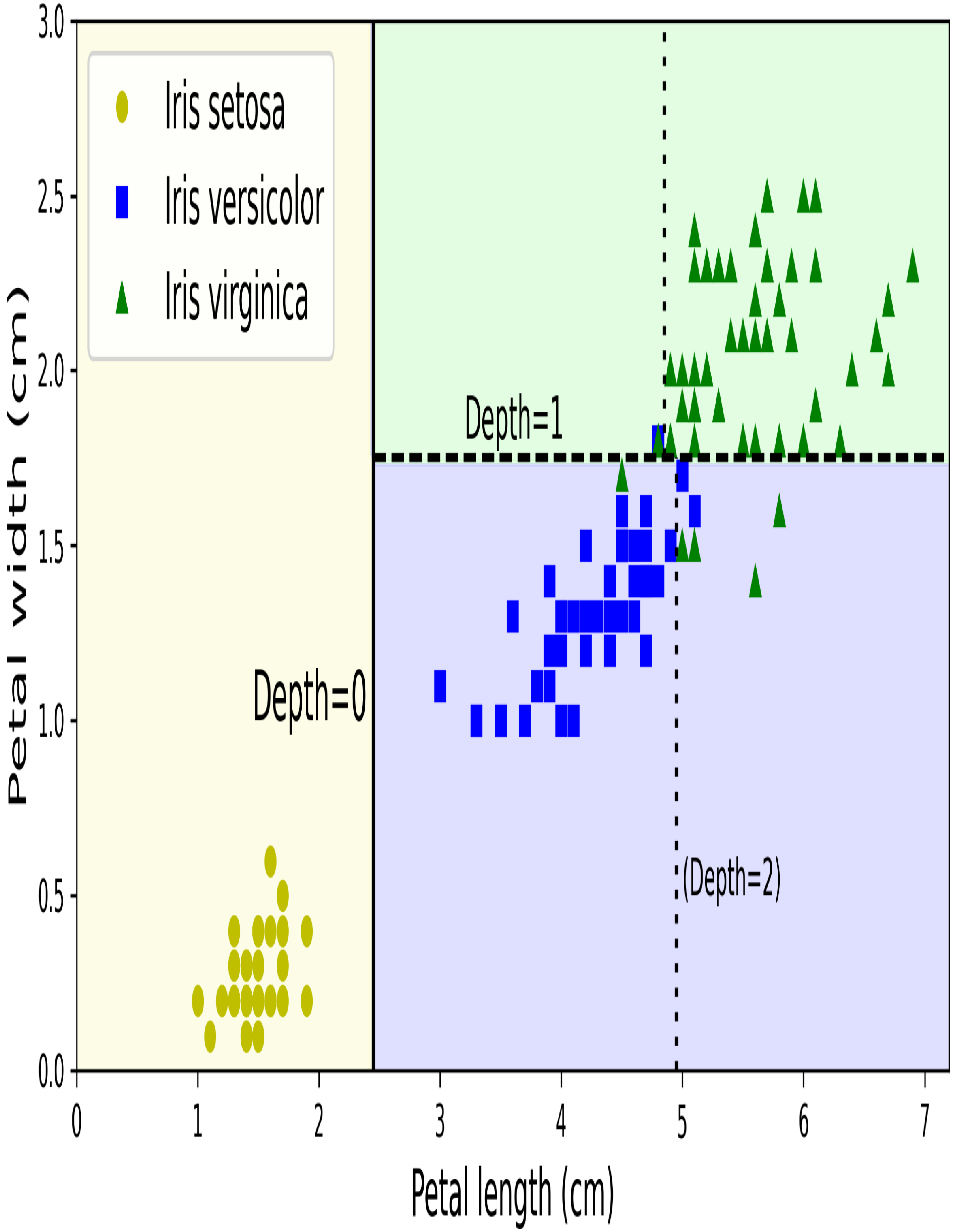


Figure 6-2. Decision Tree decision boundaries

MODEL INTERPRETATION: WHITE BOX VERSUS BLACK BOX

Decision Trees are intuitive, and their decisions are easy to interpret. Such models are often called *white box models*. In contrast, as we will see, Random Forests or neural networks are generally considered *black box models*. They make great predictions, and you can easily check the calculations that they performed to make these predictions; nevertheless, it is usually hard to explain in simple terms why the predictions were made. For example, if a neural network says that a particular person appears on a picture, it is hard to know what contributed to this prediction: did the model recognize that person's eyes? Their mouth? Their nose? Their shoes? Or even the couch that they were sitting on? Conversely, Decision Trees provide nice, simple classification rules that can even be applied manually if need be (e.g., for flower classification). The field of *Interpretable ML* aims at creating ML systems that can explain their decisions in a way humans can understand. This is important in many domains, for example to ensure the system does not make unfair decisions.

TIP

The tree structure, including all the information shown in Figure 6-1, is available via the classifier's `tree_` attribute. Type `help(tree_clf.tree_)` for details, and see the notebook for an example.

Estimating Class Probabilities

A Decision Tree can also estimate the probability that an instance belongs to a particular class *k*. First it traverses the tree to find the leaf node for this instance, and then it returns the ratio of training instances of class *k* in this node. For example, suppose you have found a flower whose petals are 5 cm long and 1.5 cm wide. The corresponding leaf node is the depth-2 left node, so the Decision Tree outputs the following probabilities: 0% for *Iris setosa* (0/54), 90.7% for *Iris versicolor* (49/54), and 9.3% for *Iris virginica* (5/54). And if you ask it to predict the class, it outputs *Iris versicolor* (class 1) because it has the highest probability. Let's check this:

```
>>> tree_clf.predict_proba([[5, 1.5]]).round(3)
array([[0.    , 0.907, 0.093]])
>>> tree_clf.predict([[5, 1.5]])
array([1])
```

Perfect! Notice that the estimated probabilities would be identical anywhere else in the bottom-right rectangle of Figure 6-2—for example, if the petals were 6 cm long and 1.5 cm wide (even though it seems obvious that it would most likely be an *Iris virginica* in this case).

The CART Training Algorithm

Scikit-Learn uses the *Classification and Regression Tree* (CART) algorithm to train Decision Trees (also called "growing" trees). The algorithm works by first splitting the training set into two subsets using a single feature k and a threshold t_k (e.g., "petal length ≤ 2.45 cm"). How does it choose k and t_k? It searches for the pair (k, t_k) that produces the purest subsets, weighted by their size. Equation 6-2 gives the cost function that the algorithm tries to minimize.

Equation 6-2. CART cost function for classification

$$J(k, t_k) = \frac{m_{\text{left}}}{m} G_{\text{left}} + \frac{m_{\text{right}}}{m} G_{\text{right}}$$
$$\text{where} \begin{cases} G_{\text{left/right}} \text{ measures the impurity of the left/right subset,} \\ m_{\text{left/right}} \text{ is the number of instances in the left/right subset.} \end{cases}$$

Once the CART algorithm has successfully split the training set in two, it splits the subsets using the same logic, then the sub-subsets, and so on, recursively. It stops recursing once it reaches the maximum depth (defined by the `max_depth` hyperparameter), or if it cannot find a split that will reduce impurity. A few other hyperparameters (described in a moment) control additional stopping conditions: `min_samples_split`, `min_samples_leaf`, `min_weight_fraction_leaf`, and `max_leaf_nodes`.

> **WARNING**
>
> As you can see, the CART algorithm is a *greedy algorithm*: it greedily searches for an optimum split at the top level, then repeats the process at each subsequent level. It does not check whether or not the split will lead to the lowest possible impurity several levels down. A greedy algorithm often produces a solution that's reasonably good but not guaranteed to be optimal.
>
> Unfortunately, finding the optimal tree is known to be an *NP-Complete* problem.[1] It requires O(exp(m)) time, making the problem intractable even for small training sets. This is why we must settle for a "reasonably good" solution when training decision trees.

Computational Complexity

Making predictions requires traversing the Decision Tree from the root to a leaf. Decision Trees generally are approximately balanced, so traversing the Decision Tree requires going through roughly ڽ□og$_2$(m)) nodes, where $\log_2(m)$ is the *binary logarithm* of m, equal to $\log(m)$ / $\log(2)$. Since each node only requires checking the value of one feature, the overall prediction complexity is ڽ□og$_2$(m)), independent of the number of features. So predictions are very fast, even when dealing with large training sets.

The training algorithm compares all features (or less if `max_features` is set) on all samples at each node. Comparing all features on all samples at each node results in a training complexity of ڽ□n_ × $m \log_2(m)$).

Gini Impurity or Entropy?

By default, the `DecisionTreeClassifier` class uses the Gini impurity measure, but you can select the *entropy* impurity measure instead by setting the `criterion` hyperparameter to `"entropy"`. The concept of entropy originated in thermodynamics as a measure of molecular disorder: entropy approaches zero when molecules are still and well ordered. Entropy later spread to a wide variety of domains, including in Shannon's information theory, where it measures the average information content of a message, as we saw in Chapter 4. Entropy is zero when all messages are identical. In Machine Learning, entropy is frequently used as an impurity measure: a set's entropy is zero when it contains instances of only one class. Equation 6-3 shows the definition of the entropy of the i^{th} node. For example, the depth-2 left node in Figure 6-1 has an entropy equal to –(49/54) $\log_2$ (49/54) – (5/54) $\log_2$ (5/54) ≈ 0.445.

Equation 6-3. Entropy

$$H_i = -\sum_{\substack{k=1 \\ p_{i,k} \neq 0}}^{n} p_{i,k} \log_2 \left(p_{i,k}\right)$$

So, should you use Gini impurity or entropy? The truth is, most of the time it does not make a big difference: they lead to similar trees. Gini impurity is slightly faster to compute, so it is a good default. However, when they differ, Gini impurity tends to isolate the most frequent class in its own branch of the tree, while entropy tends to produce slightly more balanced trees.[2]

Regularization Hyperparameters

Decision Trees make very few assumptions about the training data (as opposed to linear models, which assume that the data is linear, for example). If left unconstrained, the tree structure will adapt itself to the training data, fitting it very closely—indeed, most likely overfitting it. Such a model is often called a *nonparametric model*, not because it does not have any parameters (it often has a lot) but because the number of parameters is not determined prior to training, so the model structure is free to stick closely to the data. In contrast, a *parametric model*, such as a linear model, has a predetermined number of parameters, so its degree of freedom is limited, reducing the risk of overfitting (but increasing the risk of underfitting).

To avoid overfitting the training data, you need to restrict the Decision Tree's freedom during training. As you know by now, this is called regularization. The regularization hyperparameters depend on the algorithm used, but generally you can at least restrict the maximum depth of the Decision Tree. In Scikit-Learn, this is controlled by the `max_depth` hyperparameter. The default value is `None`, which means unlimited. Reducing `max_depth` will regularize the model and thus reduce the risk of overfitting.

The `DecisionTreeClassifier` class has a few other parameters that similarly restrict the shape of the Decision Tree:

- `max_features`: maximum number of features that are evaluated for splitting at each node
- `max_leaf_nodes`: maximum number of leaf nodes
- `min_samples_split`: minimum number of samples a node must have before it can be split
- `min_samples_leaf`: minimum number of samples a leaf node must have to be created
- `min_weight_fraction_leaf`: same as `min_samples_leaf` but expressed as a fraction of the total number of weighted instances

Increasing `min_*` hyperparameters or reducing `max_*` hyperparameters will regularize the model.

> **NOTE**
>
> Other algorithms work by first training the Decision Tree without restrictions, then *pruning* (deleting) unnecessary nodes. A node whose children are all leaf nodes is considered unnecessary if the purity improvement it provides is not statistically significant. Standard statistical tests, such as the χ^2 *test* (chi-squared test), are used to estimate the probability that the improvement is purely the result of chance (which is called the *null hypothesis*). If this probability, called the *p-value*, is higher than a given threshold (typically 5%, controlled by a hyperparameter), then the node is considered unnecessary and its children are deleted. The pruning continues until all unnecessary nodes have been pruned.

Let's test regularization on the *moons dataset*, introduced in Chapter 5. We'll train one decision tree without regularization, and another with `min_samples_leaf=5`. Figure 6-3 shows the decision boundaries of each tree.

```
from sklearn.datasets import make_moons

X_moons, y_moons = make_moons(n_samples=150, noise=0.2, random_state=42)

tree_clf1 = DecisionTreeClassifier(random_state=42)
tree_clf2 = DecisionTreeClassifier(min_samples_leaf=5, random_state=42)
tree_clf1.fit(X_moons, y_moons)
tree_clf2.fit(X_moons, y_moons)
```

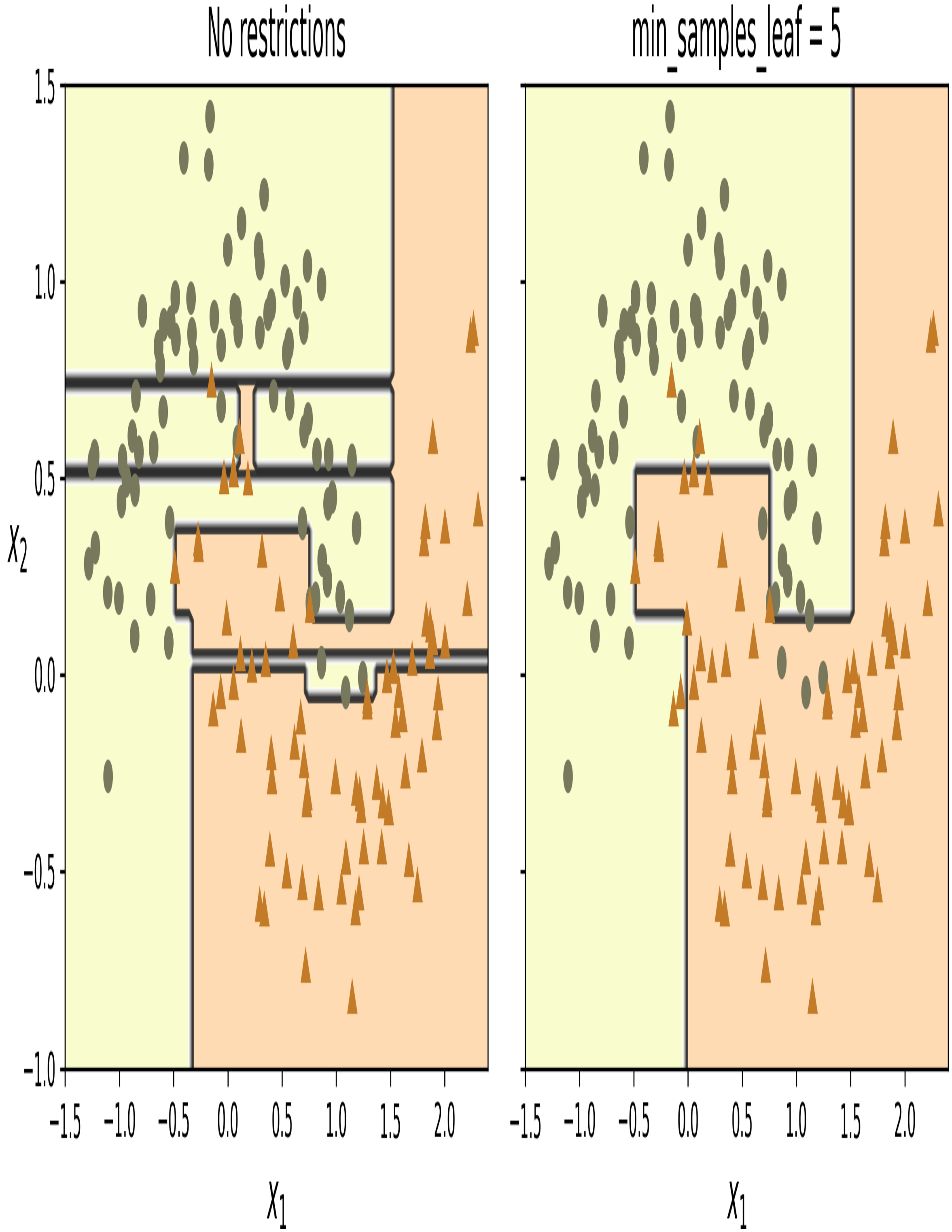


Figure 6-3. Decision boundaries of an unregularized tree (left) and a regularized tree (right)

The unregularized model on the left is clearly overfitting, and the regularized model on the right will probably generalize better. We can verify this by evaluating both trees on a test set generated using a different random seed:

```
>>> X_moons_test, y_moons_test = make_moons(n_samples=1000, noise=0.2,
...                                         random_state=43)
...
>>> tree_clf1.score(X_moons_test, y_moons_test)
0.898
>>> tree_clf2.score(X_moons_test, y_moons_test)
0.92
```

Indeed, the second tree has a better accuracy on the test set.

Regression

Decision Trees are also capable of performing regression tasks. Let's build a regression tree using Scikit-Learn's `DecisionTreeRegressor` class, training it on a noisy quadratic dataset with `max_depth=2`:

```
import numpy as np
from sklearn.tree import DecisionTreeRegressor

np.random.seed(42)
X_quad = np.random.rand(200, 1) - 0.5  # a single random input feature
y_quad = X_quad ** 2 + 0.025 * np.random.randn(200, 1)

tree_reg = DecisionTreeRegressor(max_depth=2, random_state=42)
tree_reg.fit(X_quad, y_quad)
```

The resulting tree is represented in Figure 6-4.

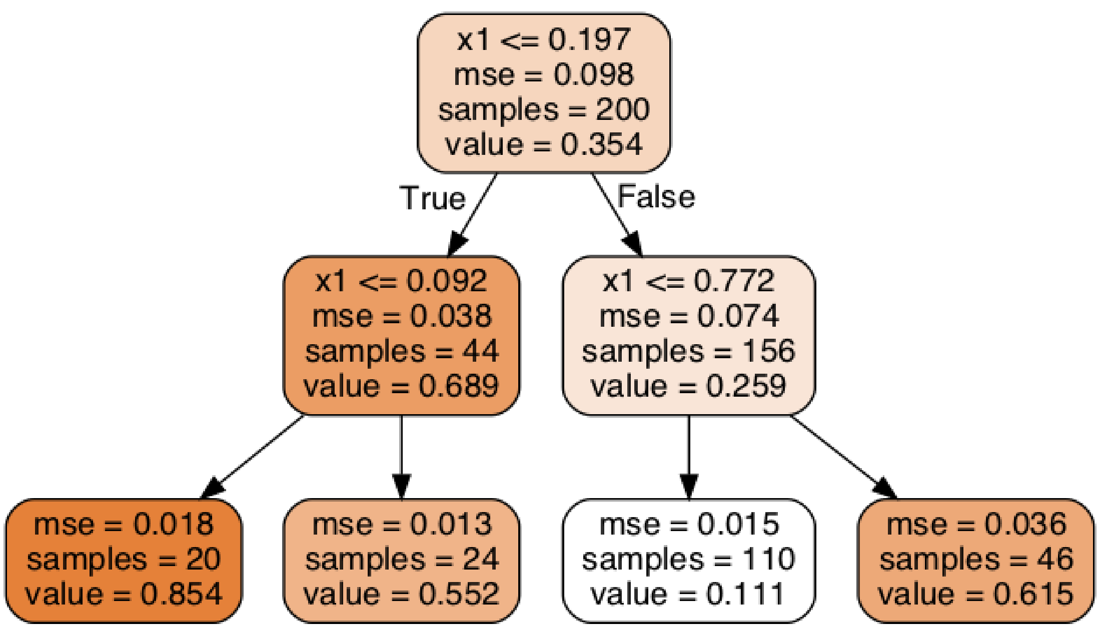


Figure 6-4. A Decision Tree for regression

This tree looks very similar to the classification tree you built earlier. The main difference is that instead of predicting a class in each node, it predicts a value. For example, suppose you want to make a prediction for a new instance with $x_1 = 0.2$. The root node asks whether $x_1 \leq 0.197$. Since it is not, the algorithm goes to the right child node, which asks whether $x_1 \leq 0.772$. Since it is, the algorithm goes to the left child node. This is a leaf node, and it predicts `value=0.111`. This prediction is the average target value of the 110 training instances associated with this leaf node, and it results in a mean squared error equal to 0.015 over these 110 instances.

This model's predictions are represented on the left in Figure 6-5. If you set `max_depth=3`, you get the predictions represented on the right. Notice how the predicted value for each region is always the average target value of the instances in that region. The algorithm splits each region in a way that makes most training instances as close as possible to that predicted value.

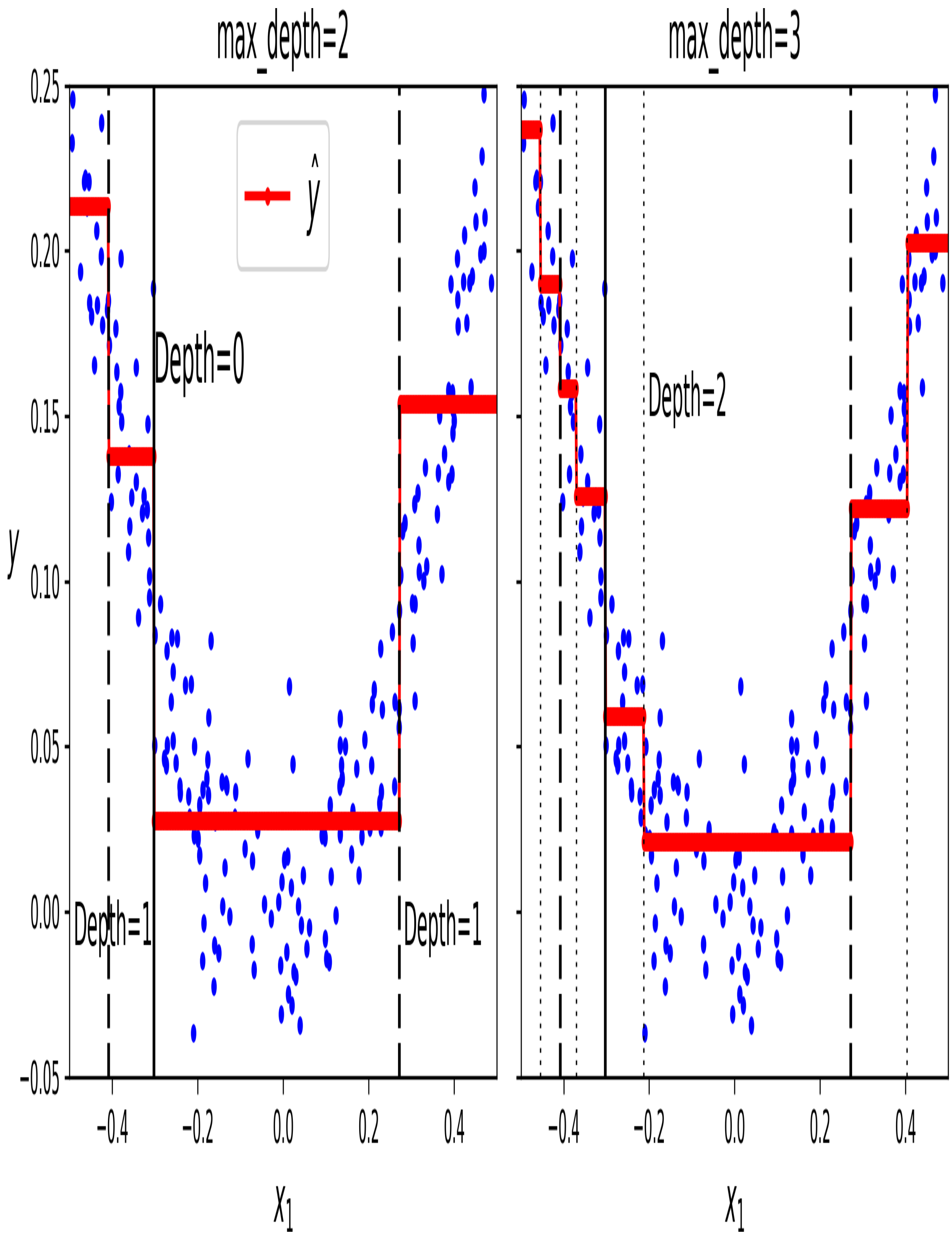


Figure 6-5. Predictions of two Decision Tree regression models

The CART algorithm works mostly the same way as earlier, except that instead of trying to split the training set in a way that minimizes impurity, it now tries to split the training set in a way that minimizes the MSE. Equation 6-4 shows the cost function that the algorithm tries to minimize.

Equation 6-4. CART cost function for regression

$$J\left(k, t_k\right) = \frac{m_{\text{left}}}{m}\text{MSE}_{\text{left}} + \frac{m_{\text{right}}}{m}\text{MSE}_{\text{right}} \quad \text{where} \begin{cases} \text{MSE}_{\text{node}} = \frac{\sum_{i \in \text{node}} \left(\hat{y}_{\text{node}} - y^{(i)}\right)^2}{m_{\text{node}}} \\ \hat{y}_{\text{node}} = \frac{\sum_{i \in \text{node}} y^{(i)}}{m_{\text{node}}} \end{cases}$$

Just like for classification tasks, Decision Trees are prone to overfitting when dealing with regression tasks. Without any regularization (i.e., using the default hyperparameters), you get the predictions on the left in Figure 6-6. These predictions are obviously overfitting the training set very badly. Just setting `min_samples_leaf=10` results in a much more reasonable model, represented on the right in Figure 6-6.

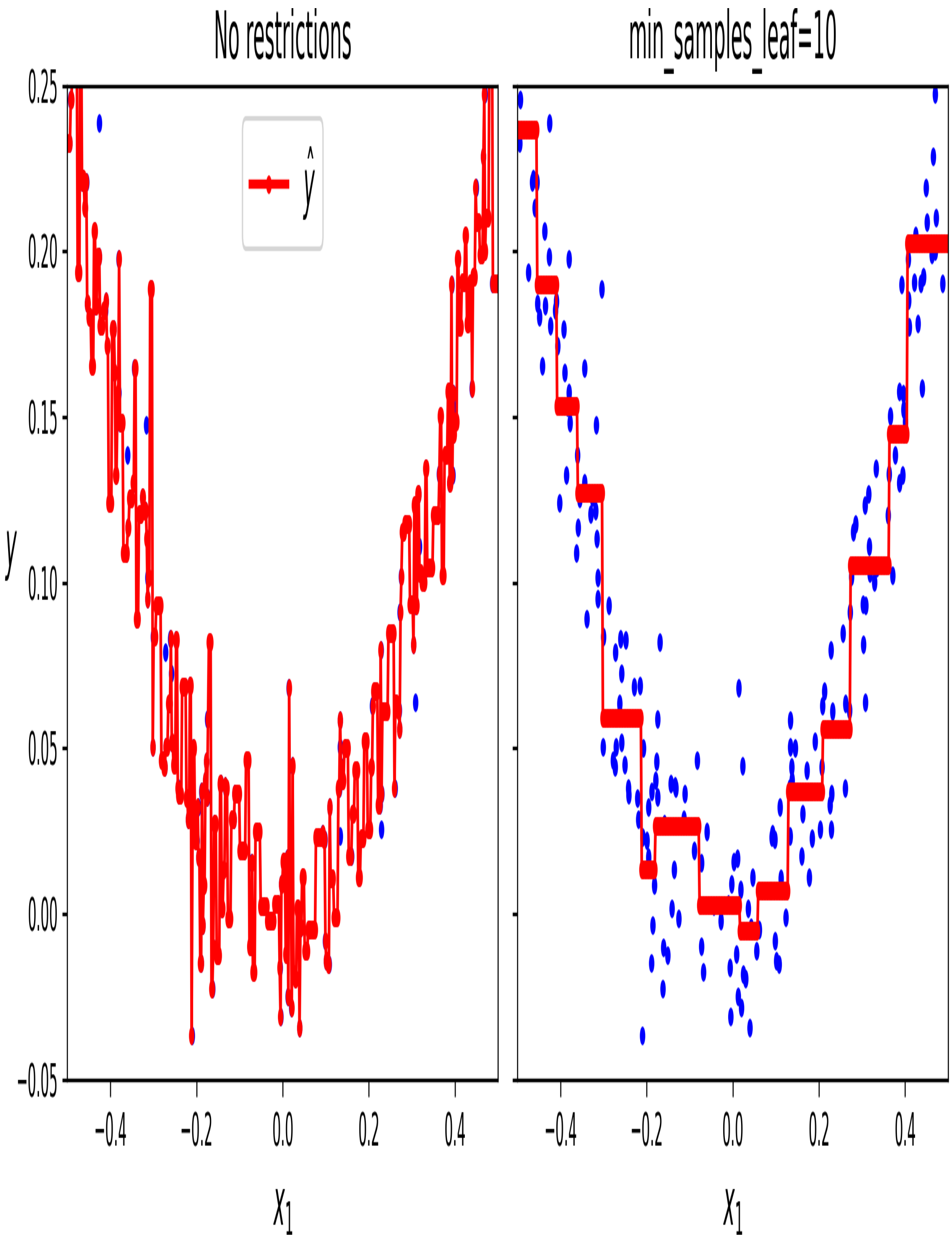


Figure 6-6. Predictions of an unregularized regression tree (left) and a regularized tree (right)

Sensitivity to axis orientation

Hopefully by now you are convinced that Decision Trees have a lot going for them: they are relatively easy to understand and interpret, simple to use, versatile, and powerful. However, they do have a few limitations. First, as you may have noticed, Decision Trees love orthogonal decision boundaries (all splits are perpendicular to an axis), which makes them sensitive to the data's orientation. For example, Figure 6-7 shows a simple linearly separable dataset: on the left, a Decision Tree can split it easily, while on the right, after the dataset is rotated by 45°, the decision boundary looks unnecessarily convoluted. Although both Decision Trees fit the training set perfectly, it is very likely that the model on the right will not generalize well.

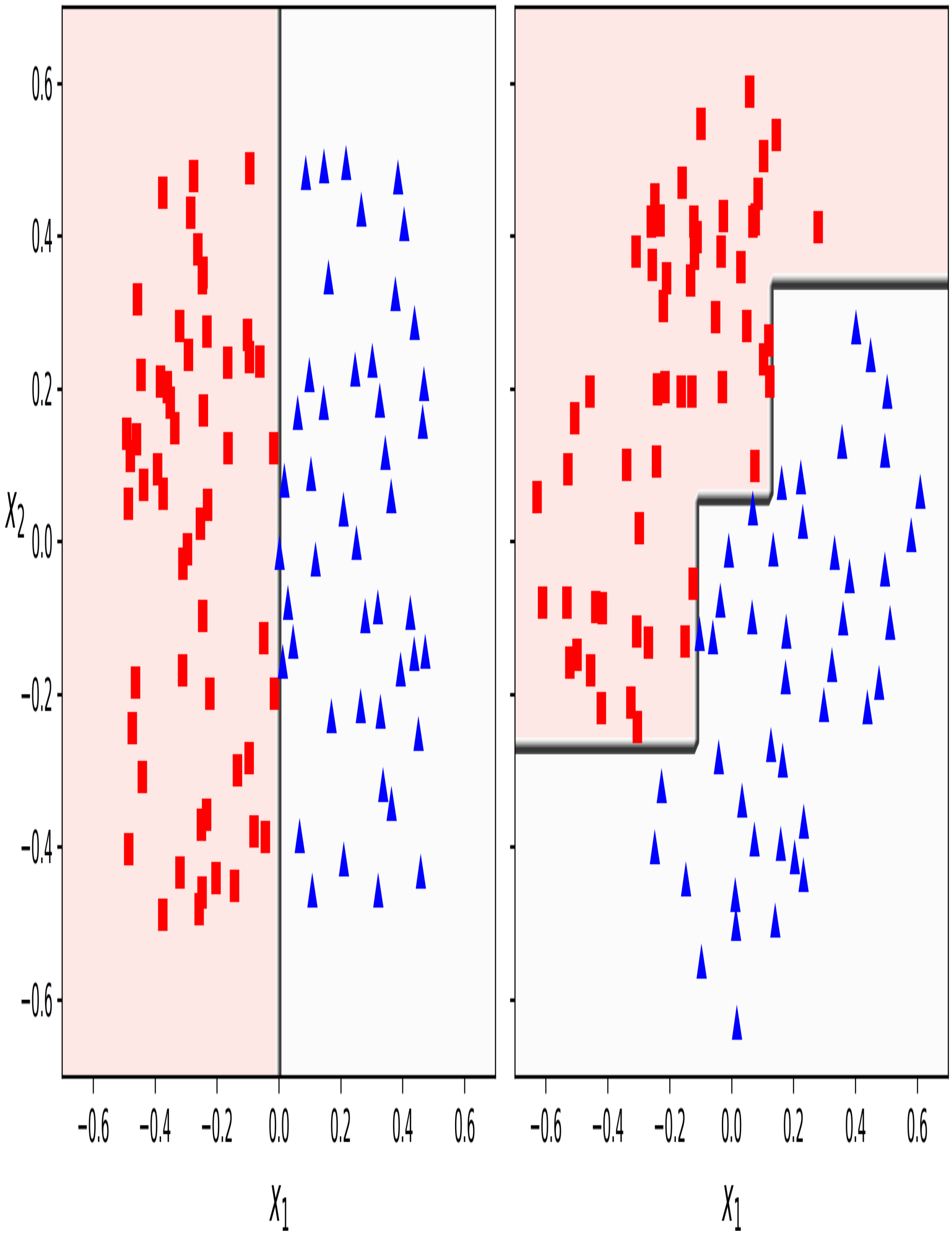


Figure 6-7. Sensitivity to training set rotation

One way to limit this problem is to scale the data then apply a Principal Component Analysis tranformation. We will look at PCA in detail in Chapter 8, but for now you only need to know that it rotates the data in a way that reduces the correlation between the features, which often (not always) makes things easier for trees. Let's create a small pipeline that scales the data and rotates it using PCA, then let's train a `DecisionTreeClassifier` on that data. Figure 6-8 shows the decision boundaries of that tree: as you can see, the rotation makes it possible to fit the dataset pretty well using only one feature, z_1, which is a linear function of the original petal length and width.

```
from sklearn.decomposition import PCA
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler

pca_pipeline = make_pipeline(StandardScaler(), PCA())
X_iris_rotated = pca_pipeline.fit_transform(X_iris)
tree_clf_pca = DecisionTreeClassifier(max_depth=2, random_state=42)
tree_clf_pca.fit(X_iris_rotated, y_iris)
```

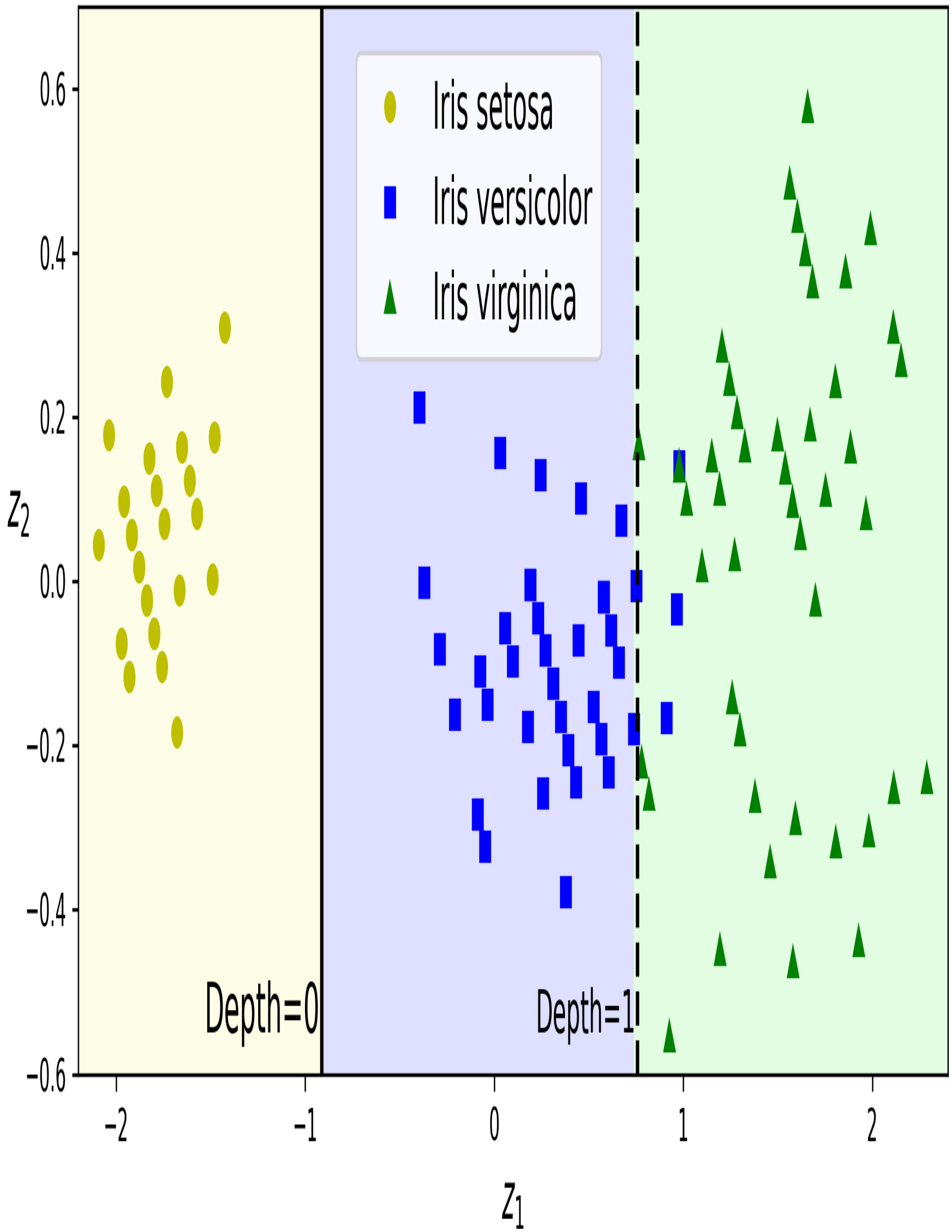


Figure 6-8. A tree's decision boundaries on the scaled and PCA-rotated iris dataset

Decision Trees have a high variance

More generally, the main issue with Decision Trees is that they have quite a high variance: small changes to the hyperparameters or to the data may produce very different models. In fact, since the training algorithm used by Scikit-Learn is stochastic—it randomly selects the set of features to evaluate at each node—even retraining the same Decision Tree on the exact same data may produce a very different model, such as the one represented in Figure 6-9 (unless you set the `random_state` hyperparameter). As you can see, it looks very different from the previous Decision Tree (Figure 6-2).

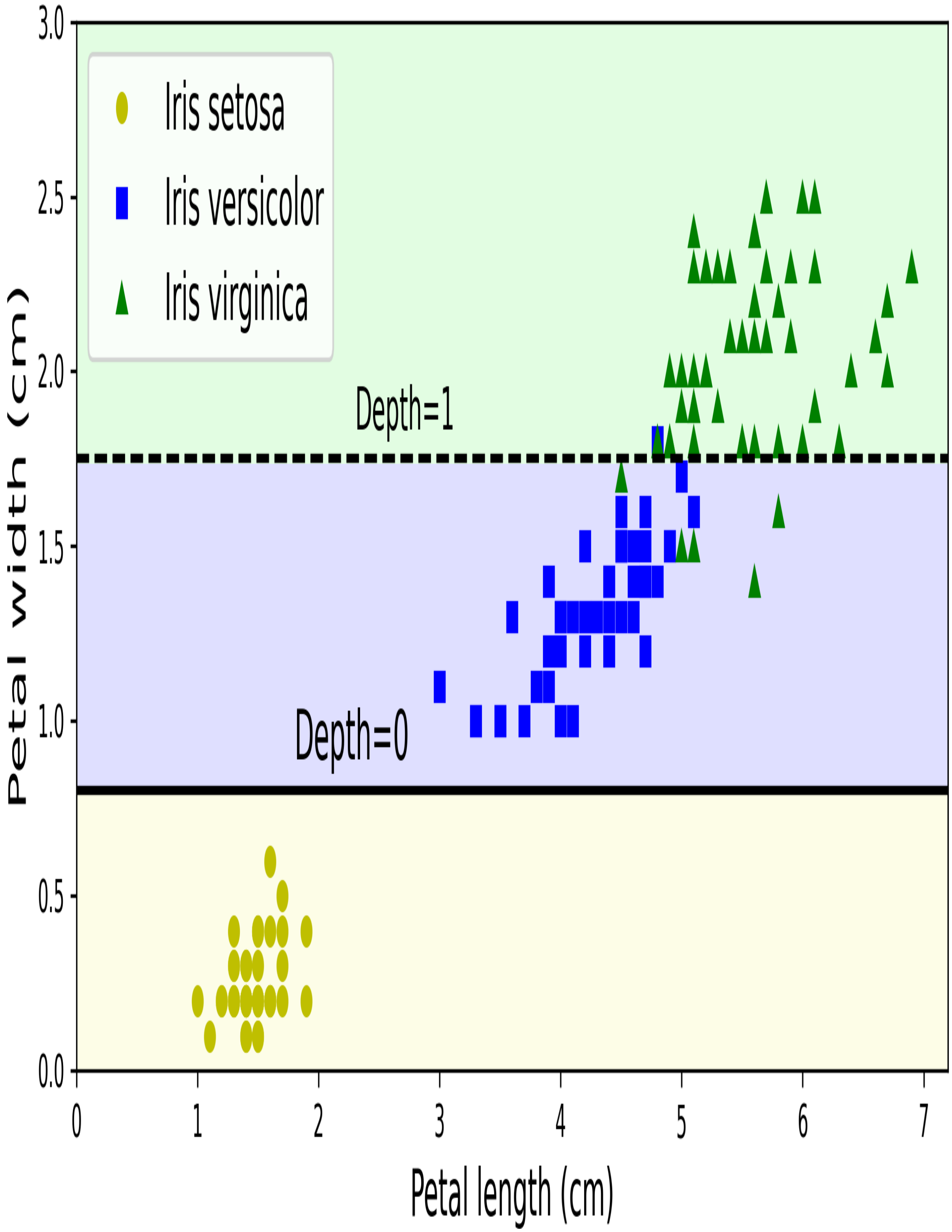


Figure 6-9. Retraining the same model on the same data may produce a very different model

Luckily, by averaging predictions over many trees, it's possible to reduce variance significantly. Such an *ensemble* of trees is called a *Random Forest*, and it's one of the most powerful types of models available today, as we will see in the next chapter.

Exercises

1. What is the approximate depth of a Decision Tree trained (without restrictions) on a training set with one million instances?
2. Is a node's Gini impurity generally lower or greater than its parent's? Is it *generally* lower/greater, or *always* lower/greater?
3. If a Decision Tree is overfitting the training set, is it a good idea to try decreasing `max_depth`?
4. If a Decision Tree is underfitting the training set, is it a good idea to try scaling the input features?
5. If it takes one hour to train a Decision Tree on a training set containing 1 million instances, roughly how much time will it take to train another Decision Tree on a training set containing 10 million instances? Hint: consider the CART algorithm's computational complexity.
6. If it takes one hour to train a Decision Tree on a given training set, roughly how much time will it take if you double the number of features?
7. Train and fine-tune a Decision Tree for the moons dataset by following these steps:
    a. Use `make_moons(n_samples=10000, noise=0.4)` to generate a moons dataset.
    b. Use `train_test_split()` to split the dataset into a training set and a test set.
    c. Use grid search with cross-validation (with the help of the `GridSearchCV` class) to find good hyperparameter values for a `DecisionTreeClassifier`. Hint: try various values for `max_leaf_nodes`.
    d. Train it on the full training set using these hyperparameters, and measure your model's performance on the test set. You should get roughly 85% to 87% accuracy.
8. Grow a forest by following these steps:
    a. Continuing the previous exercise, generate 1,000 subsets of the training set, each containing 100 instances selected randomly. Hint:

you can use Scikit-Learn's `ShuffleSplit` class for this.

b. Train one Decision Tree on each subset, using the best hyperparameter values found in the previous exercise. Evaluate these 1,000 Decision Trees on the test set. Since they were trained on smaller sets, these Decision Trees will likely perform worse than the first Decision Tree, achieving only about 80% accuracy.

c. Now comes the magic. For each test set instance, generate the predictions of the 1,000 Decision Trees, and keep only the most frequent prediction (you can use SciPy's `mode()` function for this). This approach gives you *majority-vote predictions* over the test set.

d. Evaluate these predictions on the test set: you should obtain a slightly higher accuracy than your first model (about 0.5 to 1.5% higher). Congratulations, you have trained a Random Forest classifier!

Solutions to these exercises are available at the end of this chapter's notebook, at *https://homl.info/colab3*.

---

1 P is the set of problems that can be solved in *polynomial time* (i.e., a polynomial of the dataset size). NP is the set of problems whose solutions can be verified in polynomial time. An NP-Hard problem is a problem that can be reduced to a known NP-Hard problem in polynomial time. An NP-Complete problem is both NP and NP-Hard. A major open mathematical question is whether or not P = NP. If P ≠ NP (which seems likely), then no polynomial algorithm will ever be found for any NP-Complete problem (except perhaps one day on a quantum computer).

2 See Sebastian Raschka's interesting analysis for more details.

Chapter 7. Ensemble Learning and Random Forests

A NOTE FOR EARLY RELEASE READERS

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.

This will be the 7th chapter of the final book. Notebooks are available on GitHub at *https://github.com/ageron/handson-ml3*. Datasets are available at *https://github.com/ageron/data*.

If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the editoor at ntache@oreilly.com.

Suppose you pose a complex question to thousands of random people, then aggregate their answers. In many cases you will find that this aggregated answer is better than an expert's answer. This is called the *wisdom of the crowd*. Similarly, if you aggregate the predictions of a group of predictors (such as classifiers or regressors), you will often get better predictions than with the best individual predictor. A group of predictors is called an *ensemble*; thus, this technique is called *Ensemble Learning*, and an Ensemble Learning algorithm is called an *Ensemble method*.

As an example of an Ensemble method, you can train a group of Decision Tree classifiers, each on a different random subset of the training set. To make predictions, you obtain the predictions of all the individual trees, then predict the class that gets the most votes (see the last exercise in Chapter 6). Such an ensemble of Decision Trees is called a *Random Forest*, and despite its simplicity, this is one of the most powerful Machine Learning algorithms available today.

As discussed in Chapter 2, you will often use Ensemble methods near the end of a project, once you have already built a few good predictors, to combine them into an even better predictor. In fact, the winning solutions in Machine Learning competitions often involve several Ensemble methods—most famously in the Netflix Prize competition.

In this chapter we will discuss the most popular Ensemble methods, including *bagging*, *boosting*, and *stacking*. We will also explore Random Forests.

Voting Classifiers

Suppose you have trained a few classifiers, each one achieving about 80% accuracy. You may have a Logistic Regression classifier, an SVM classifier, a Random Forest classifier, a K-Nearest Neighbors classifier, and perhaps a few more (see Figure 7-1).

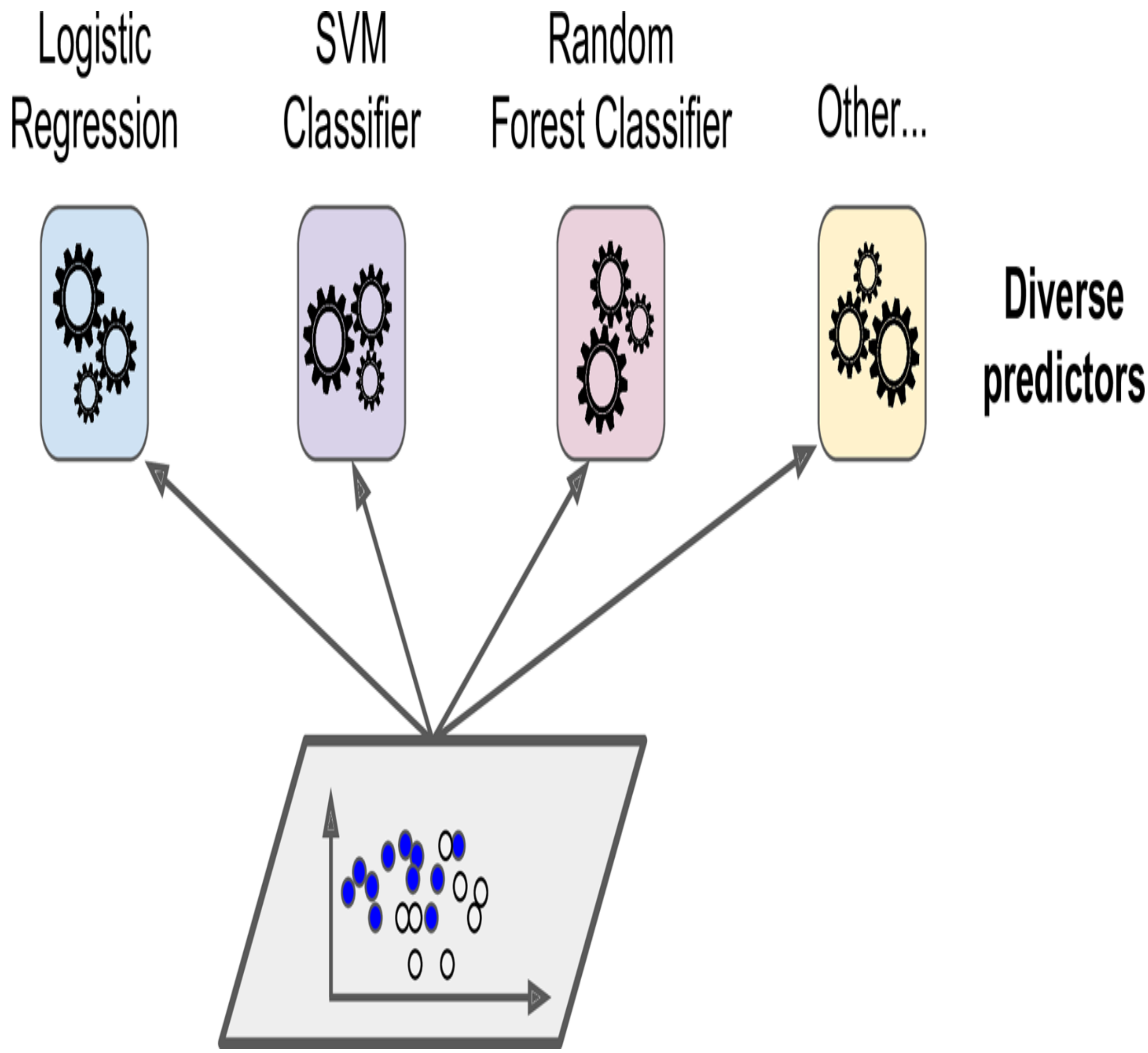


Figure 7-1. Training diverse classifiers

A very simple way to create an even better classifier is to aggregate the predictions of each classifier and predict the class that gets the most votes. This majority-vote classifier is called a *hard voting* classifier (see Figure 7-2).

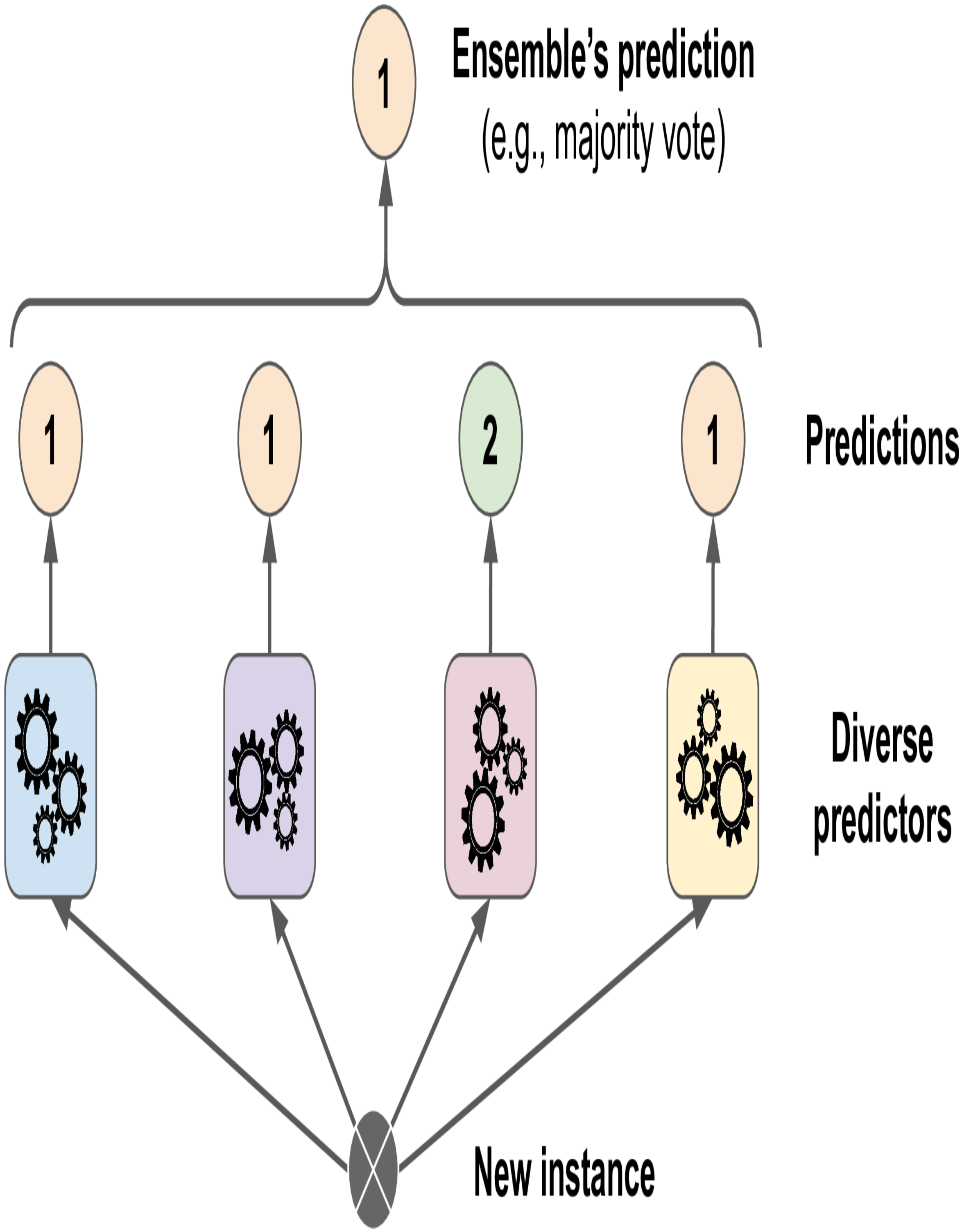


Figure 7-2. Hard voting classifier predictions

Somewhat surprisingly, this voting classifier often achieves a higher accuracy than the best classifier in the ensemble. In fact, even if each classifier is a *weak learner* (meaning it does only slightly better than random guessing), the ensemble can still be a *strong* *learner* (achieving high accuracy), provided there are a sufficient number of weak learners and they are sufficiently diverse.

How is this possible? The following analogy can help shed some light on this mystery. Suppose you have a slightly biased coin that has a 51% chance of coming up heads and 49% chance of coming up tails. If you toss it 1,000 times, you will generally get more or less 510 heads and 490 tails, and hence a majority of heads. If you do the math, you will find that the probability of obtaining a majority of heads after 1,000 tosses is close to 75%. The more you toss the coin, the higher the probability (e.g., with 10,000 tosses, the probability climbs over 97%). This is due to the *law of large numbers*: as you keep tossing the coin, the ratio of heads gets closer and closer to the probability of heads (51%). Figure 7-3 shows 10 series of biased coin tosses. You can see that as the number of tosses increases, the ratio of heads approaches 51%. Eventually all 10 series end up so close to 51% that they are consistently above 50%.

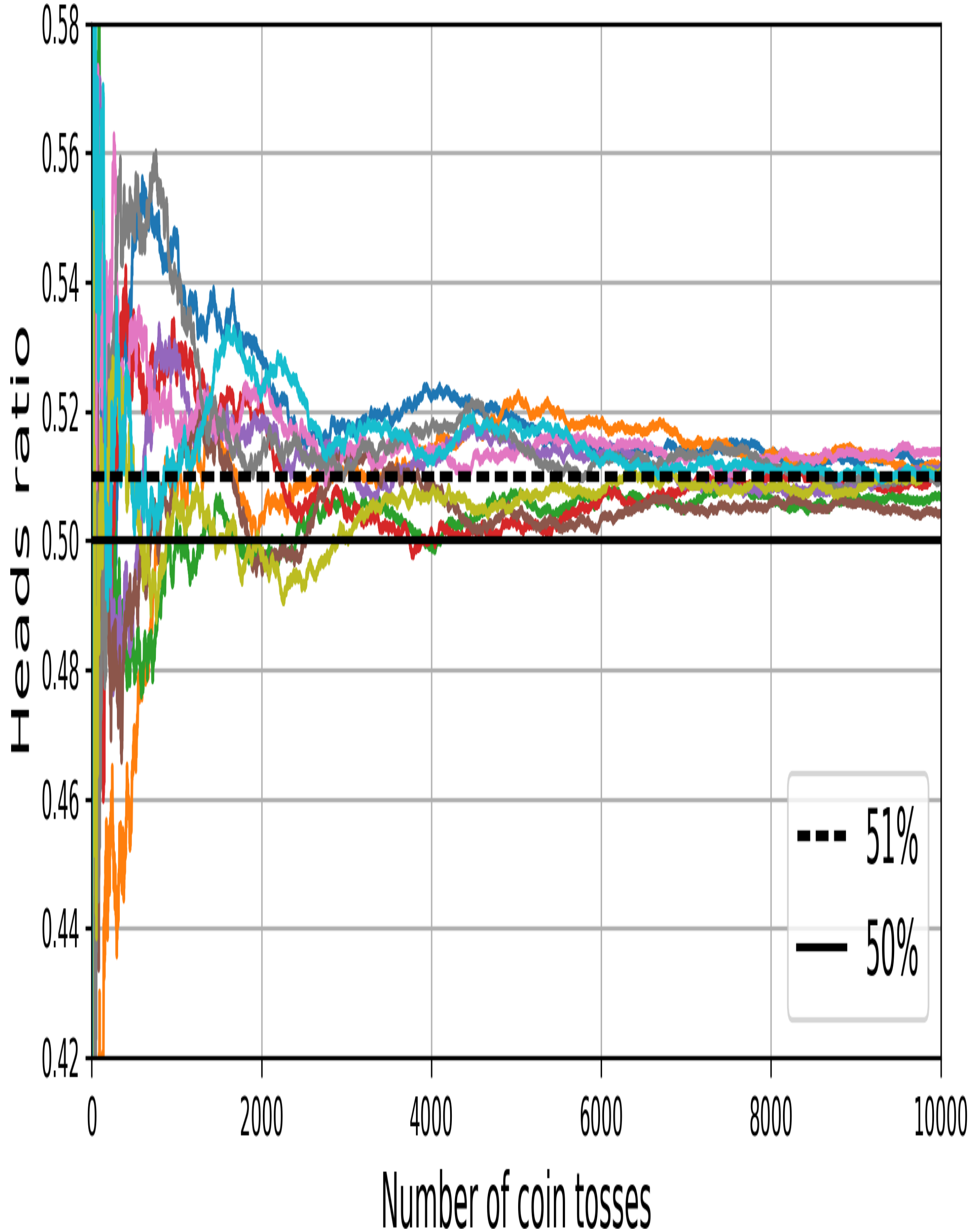


Figure 7-3. The law of large numbers

Similarly, suppose you build an ensemble containing 1,000 classifiers that are individually correct only 51% of the time (barely better than random guessing). If you predict the majority voted class, you can hope for up to 75% accuracy! However, this is only true if all classifiers are perfectly independent, making uncorrelated errors, which is clearly not the case because they are trained on the same data. They are likely to make the same types of errors, so there will be many majority votes for the wrong class, reducing the ensemble's accuracy.

> **TIP**
>
> Ensemble methods work best when the predictors are as independent from one another as possible. One way to get diverse classifiers is to train them using very different algorithms. This increases the chance that they will make very different types of errors, improving the ensemble's accuracy.

Scikit-Learn provides a `VotingClassifier` class that's quite easy to use: just give it a list of name/predictor pairs, and use it like a normal classifier, that's it! Let's try it on the moons dataset (introduced in Chapter 6): we will load and split the moons dataset into a training set and a test set, then we'll create and train a voting classifier composed of three diverse classifiers:

```
from sklearn.datasets import make_moons
from sklearn.ensemble import RandomForestClassifier, VotingClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import train_test_split
from sklearn.svm import SVC

X, y = make_moons(n_samples=500, noise=0.30, random_state=42)
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=42)

voting_clf = VotingClassifier(
    estimators=[
        ('lr', LogisticRegression(random_state=42)),
        ('rf', RandomForestClassifier(random_state=42)),
        ('svc', SVC(random_state=42))
    ]
)
voting_clf.fit(X_train, y_train)
```

When you fit a `VotingClassifier`, it clones every estimator and fits the clones. The original estimators are available via the `estimators` attribute, while the fitted clones are available via the `estimators_` attribute. If you prefer a dict rather than a list, you can use `named_estimators` or `named_estimators_` instead. For example, let's look at each fitted classifier's accuracy on the test set:

```
>>> for name, clf in voting_clf.named_estimators_.items():
...     print(name, "=", clf.score(X_test, y_test))
...
lr = 0.864
```

```
rf = 0.896
svc = 0.896
```

When you call the voting classifier's `predict()` method, it performs hard voting. For example, the voting classifier predicts class 1 for the first instance of the test set, because 2 out of 3 classifiers predict that class:

```
>>> voting_clf.predict(X_test[:1])
array([1])
>>> [clf.predict(X_test[:1]) for clf in voting_clf.estimators_]
[array([1]), array([1]), array([0])]
```

Now let's look at the performance of the voting classifier on the test set:

```
>>> voting_clf.score(X_test, y_test)
0.912
```

There you have it! The voting classifier outperforms all the individual classifiers.

If all classifiers are able to estimate class probabilities (i.e., they all have a `predict_proba()` method), then you can tell Scikit-Learn to predict the class with the highest class probability, averaged over all the individual classifiers. This is called *soft voting*. It often achieves higher performance than hard voting because it gives more weight to highly confident votes. All you need to do is set the voting classifier's `voting` hyperparameter to `"soft"`, and ensure that all classifiers can estimate class probabilities. This is not the case for the `SVC` class by default, so you need to set its `probability` hyperparameter to `True` (this will make the `SVC` class use cross-validation to estimate class probabilities, slowing down training, and it will add a `predict_proba()` method). Let's try that:

```
>>> voting_clf.voting = "soft"
>>> voting_clf.named_estimators["svc"].probability = True
>>> voting_clf.fit(X_train, y_train)
>>> voting_clf.score(X_test, y_test)
0.92
```

We reach 92% accuracy simply by using soft voting, not bad!

Bagging and Pasting

One way to get a diverse set of classifiers is to use very different training algorithms, as just discussed. Another approach is to use the same training algorithm for every predictor but train them on different random subsets of the training set. When sampling is performed *with* replacement, this method is called *bagging*[1] (short for *bootstrap aggregating*[2]). When sampling is performed *without* replacement, it is called *pasting*.[3]

In other words, both bagging and pasting allow training instances to be sampled several times across multiple predictors, but only bagging allows training instances to be sampled several times for the same predictor. This sampling and training process is represented in Figure 7-4.

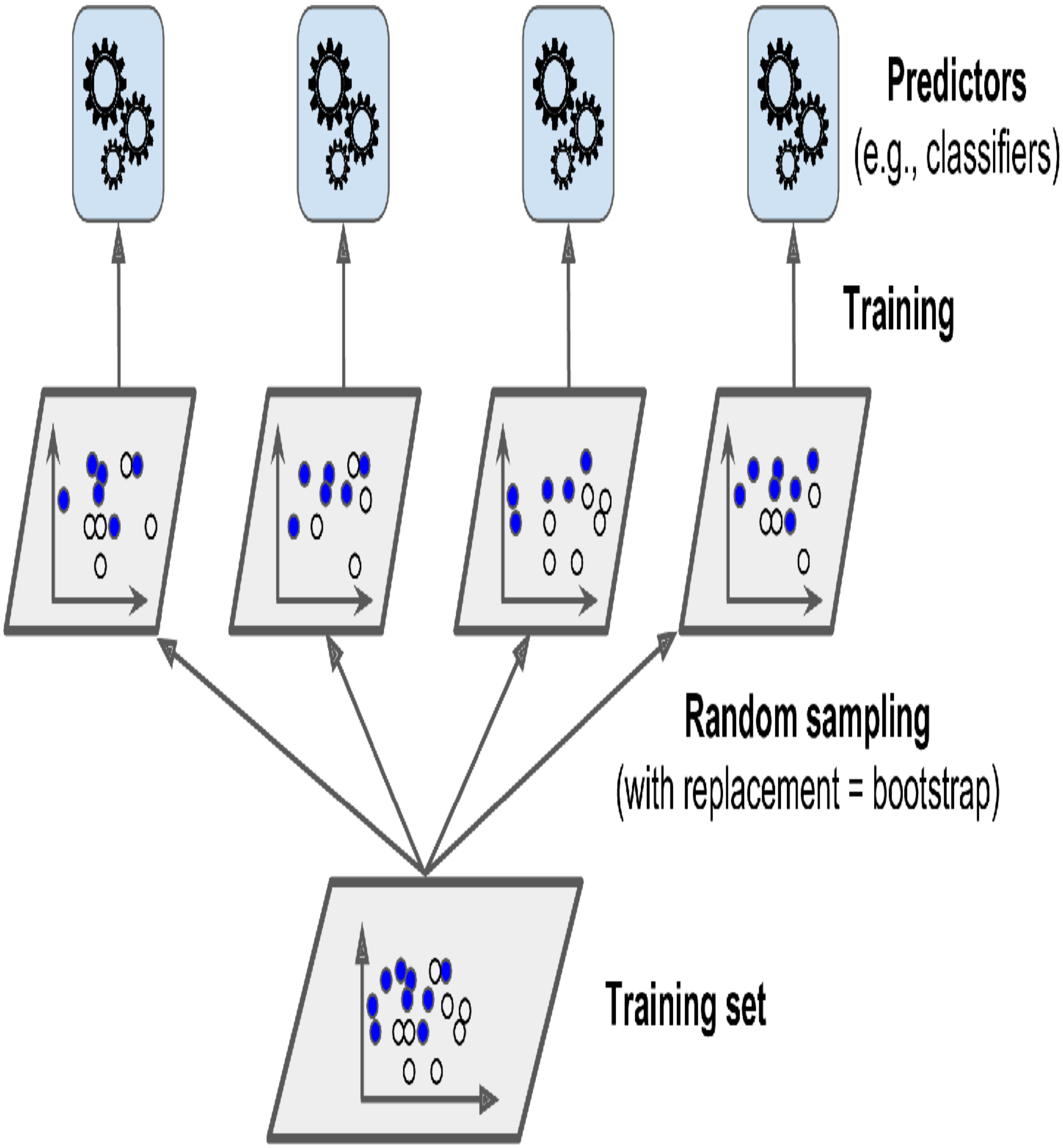


Figure 7-4. Bagging and pasting involve training several predictors on different random samples of the training set

Once all predictors are trained, the ensemble can make a prediction for a new instance by simply aggregating the predictions of all predictors. The aggregation function is typically the *statistical mode* for classification (i.e., the most frequent prediction, just like a hard voting classifier), or the average for regression. Each individual predictor has a higher bias than if it were trained on the original training set, but aggregation reduces both bias and variance.[4] Generally, the net result is that the ensemble has a similar bias but a lower variance than a single predictor trained on the original training set.

As you can see in Figure 7-4, predictors can all be trained in parallel, via different CPU cores or even different servers. Similarly, predictions can be made in parallel. This is one of the reasons bagging and pasting are such popular methods: they scale very well.

Bagging and Pasting in Scikit-Learn

Scikit-Learn offers a simple API for both bagging and pasting with the `BaggingClassifier` class (or `BaggingRegressor` for regression). The following code trains an ensemble of 500 Decision Tree classifiers:[5] each is trained on 100 training instances randomly sampled from the training set with replacement (this is an example of bagging, but if you want to use pasting instead, just set `bootstrap=False`). The `n_jobs` parameter tells Scikit-Learn the number of CPU cores to use for training and predictions, and `-1` tells Scikit-Learn to use all available cores.

```
from sklearn.ensemble import BaggingClassifier
from sklearn.tree import DecisionTreeClassifier

bag_clf = BaggingClassifier(DecisionTreeClassifier(), n_estimators=500,
                            max_samples=100, random_state=42)
bag_clf.fit(X_train, y_train)
```

> **NOTE**
>
> The `BaggingClassifier` automatically performs soft voting instead of hard voting if the base classifier can estimate class probabilities (i.e., if it has a `predict_proba()` method), which is the case with Decision Tree classifiers.

Figure 7-5 compares the decision boundary of a single Decision Tree with the decision boundary of a bagging ensemble of 500 trees (from the preceding code), both trained on the moons dataset. As you can see, the ensemble's predictions will likely generalize much better than the single Decision Tree's predictions: the ensemble has a comparable bias but a smaller variance (it makes roughly the same number of errors on the training set, but the decision boundary is less irregular).

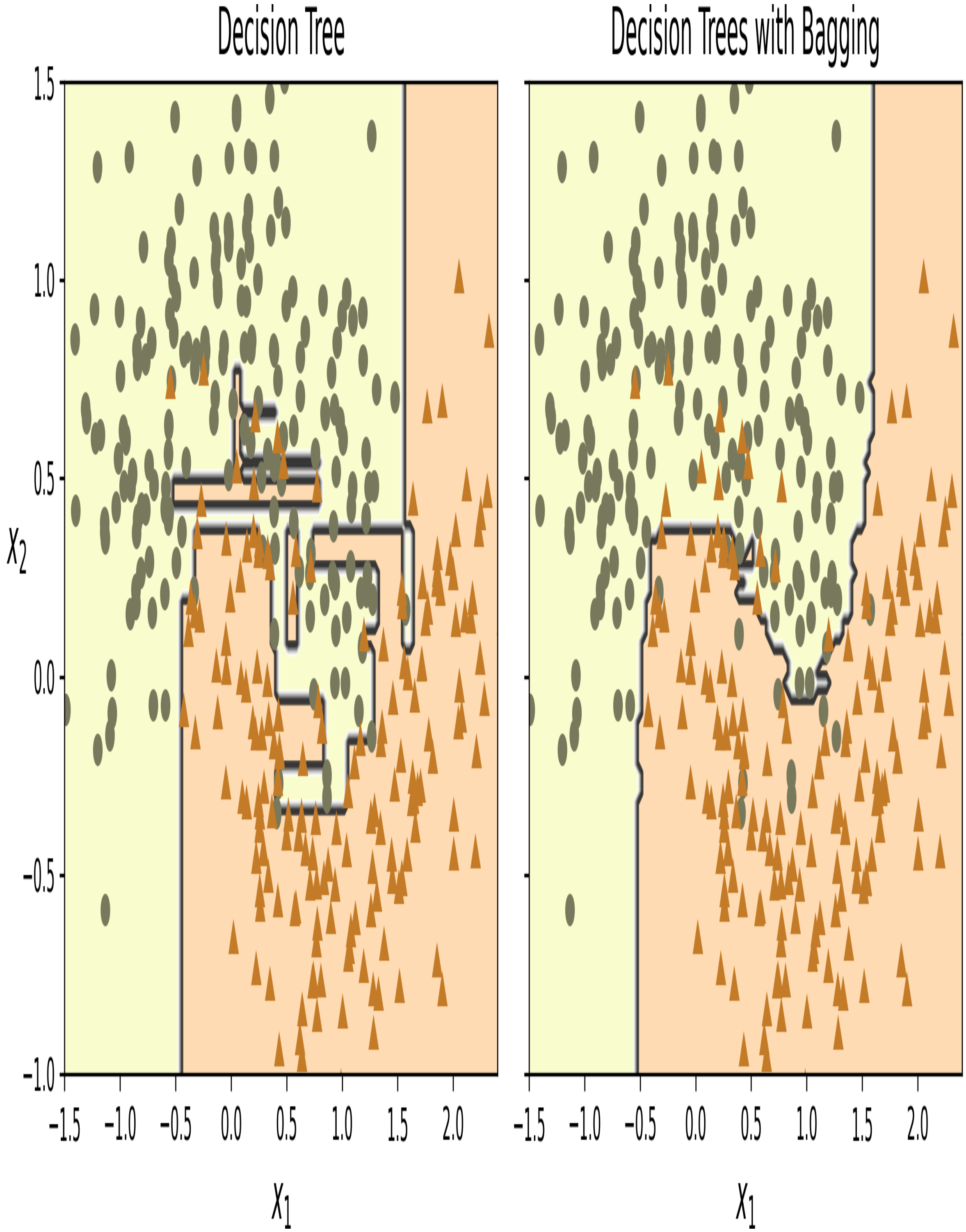


Figure 7-5. A single Decision Tree (left) versus a bagging ensemble of 500 trees (right)

Bootstrapping introduces a bit more diversity in the subsets that each predictor is trained on, so bagging ends up with a slightly higher bias than pasting; but the extra diversity also means that the predictors end up being less correlated, so the ensemble's variance is reduced. Overall, bagging often results in better models, which explains why it is generally preferred. However, if you have spare time and CPU power, you can use cross-validation to evaluate both bagging and pasting and select the one that works best.

Out-of-Bag Evaluation

With bagging, some instances may be sampled several times for any given predictor, while others may not be sampled at all. By default a `BaggingClassifier` samples *m* training instances with replacement (`bootstrap=True`), where *m* is the size of the training set. With this process, it can be shown mathematically that only about 63% of the training instances are sampled on average for each predictor.[6] The remaining 37% of the training instances that are not sampled are called *out-of-bag* (oob) instances. Note that they are not the same 37% for all predictors.

A bagging ensemble can be evaluated using oob instances, without the need for a separate validation set: indeed, if there are enough estimators, then each instance in the training set will likely be an oob instance of several estimators, so these estimators can be used to make a fair ensemble prediction for that instance. Once you have a prediction for each instance, you can compute the ensemble's prediction accuracy (or any other metric).

In Scikit-Learn, you can set `oob_score=True` when creating a `BaggingClassifier` to request an automatic oob evaluation after training. The following code demonstrates this. The resulting evaluation score is available in the `oob_score_` attribute:

```
>>> bag_clf = BaggingClassifier(DecisionTreeClassifier(), n_estimators=500,
...                             oob_score=True, random_state=42)
...
>>> bag_clf.fit(X_train, y_train)
>>> bag_clf.oob_score_
0.896
```

According to this oob evaluation, this `BaggingClassifier` is likely to achieve about 89.6% accuracy on the test set. Let's verify this:

```
>>> from sklearn.metrics import accuracy_score
>>> y_pred = bag_clf.predict(X_test)
>>> accuracy_score(y_test, y_pred)
0.92
```

We get 92% accuracy on the test. The oob evaluation was a bit too pessimistic, a bit over 2% too low.

The oob decision function for each training instance is also available through the `oob_decision_function_` attribute. Since the base estimator has a `predict_proba()` method, the decision function returns the class probabilities for each training instance. For example, the oob evaluation estimates that the first training instance has a 67.6% probability of belonging to the positive class, and 32.4% of belonging to the negative class:

```
>>> bag_clf.oob_decision_function_[:3]  # probas for the first 3 instances
array([[0.32352941, 0.67647059],
       [0.3375    , 0.6625    ],
       [1.        , 0.        ]])
```

Random Patches and Random Subspaces

The `BaggingClassifier` class supports sampling the features as well. Sampling is controlled by two hyperparameters: `max_features` and `bootstrap_features`. They work the same way as `max_samples` and `bootstrap`, but for feature sampling instead of instance sampling. Thus, each predictor will be trained on a random subset of the input features.

This technique is particularly useful when you are dealing with high-dimensional inputs (such as images). Sampling both training instances and features is called the *Random Patches* method.[7] Keeping all training instances (by setting `bootstrap=False` and `max_samples=1.0`) but sampling features (by setting `bootstrap_features` to `True` and/or `max_features` to a value smaller than `1.0`) is called the *Random Subspaces* method.[8]

Sampling features results in even more predictor diversity, trading a bit more bias for a lower variance.

Random Forests

As we have discussed, a Random Forest[9] is an ensemble of Decision Trees, generally trained via the bagging method (or sometimes pasting), typically with `max_samples` set to the size of the training set. Instead of building a `BaggingClassifier` and passing it a `DecisionTreeClassifier`, you can use the `RandomForestClassifier` class, which is more convenient and optimized for Decision Trees[10] (similarly, there is a `RandomForestRegressor` class for regression tasks). The following code trains a Random Forest classifier with 500 trees, each limited to maximum 16 nodes, and using all available CPU cores:

```python
from sklearn.ensemble import RandomForestClassifier

rnd_clf = RandomForestClassifier(n_estimators=500, max_leaf_nodes=16,
                                 n_jobs=-1, random_state=42)
rnd_clf.fit(X_train, y_train)

y_pred_rf = rnd_clf.predict(X_test)
```

With a few exceptions, a `RandomForestClassifier` has all the hyperparameters of a `DecisionTreeClassifier` (to control how trees are grown), plus all the hyperparameters of a `BaggingClassifier` to control the ensemble itself.

The Random Forest algorithm introduces extra randomness when growing trees; instead of searching for the very best feature when splitting a node (see Chapter 6), it searches for the best feature among a random subset of features. By default, it samples $\sqrt{n}$ features (where n is the total number of features). The algorithm results in greater tree diversity, which (again) trades a higher bias for a lower variance, generally yielding an overall better model. So the following `BaggingClassifier` is equivalent to the previous `RandomForestClassifier`:

```python
bag_clf = BaggingClassifier(
    DecisionTreeClassifier(max_features="sqrt", max_leaf_nodes=16),
    n_estimators=500, n_jobs=-1, random_state=42)
```

Extra-Trees

When you are growing a tree in a Random Forest, at each node only a random subset of the features is considered for splitting (as discussed earlier). It is possible to make trees even more random by also using random thresholds for each feature rather than searching for the best possible thresholds (like regular Decision Trees do). For this, simply set `splitter="random"` when creating a `DecisionTreeClassifier`.

A forest of such extremely random trees is called an *Extremely Randomized Trees* ensemble[11] (or *Extra-Trees* for short). Once again, this technique trades more bias for a lower variance. It also makes Extra-Trees much faster to train than regular Random Forests, because finding the best possible threshold for each feature at every node is one of the most time-consuming tasks of growing a tree.

You can create an Extra-Trees classifier using Scikit-Learn's `ExtraTreesClassifier` class. Its API is identical to the `RandomForestClassifier` class, except `bootstrap` defaults to `False`. Similarly, the `ExtraTreesRegressor` class has the same API as the `RandomForestRegressor` class, except `bootstrap` defaults to `False`.

TIP

It is hard to tell in advance whether a `RandomForestClassifier` will perform better or worse than an `ExtraTreesClassifier`. Generally, the only way to know is to try both and compare them using cross-validation.

Feature Importance

Yet another great quality of Random Forests is that they make it easy to measure the relative importance of each feature. Scikit-Learn measures a feature's importance by looking at how much the tree nodes that use that feature reduce impurity on average, across all trees in the forest. More precisely, it is a weighted average, where each node's weight is equal to the number of training samples that are associated with it (see Chapter 6).

Scikit-Learn computes this score automatically for each feature after training, then it scales the results so that the sum of all importances is equal to 1. You can access the result using the `feature_importances_` variable. For example, the following code trains a `RandomForestClassifier` on the iris dataset (introduced in Chapter 4) and outputs each feature's importance. It seems that the most important features are the petal length (44%) and width (42%), while sepal length and width are rather unimportant in comparison (11% and 2%, respectively):

```
>>> from sklearn.datasets import load_iris
>>> iris = load_iris(as_frame=True)
>>> rnd_clf = RandomForestClassifier(n_estimators=500, random_state=42)
>>> rnd_clf.fit(iris.data, iris.target)
>>> for score, name in zip(rnd_clf.feature_importances_, iris.data.columns):
...     print(round(score, 2), name)
...
0.11 sepal length (cm)
0.02 sepal width (cm)
0.44 petal length (cm)
0.42 petal width (cm)
```

Similarly, if you train a Random Forest classifier on the MNIST dataset (introduced in Chapter 3) and plot each pixel's importance, you get the image represented in Figure 7-6.

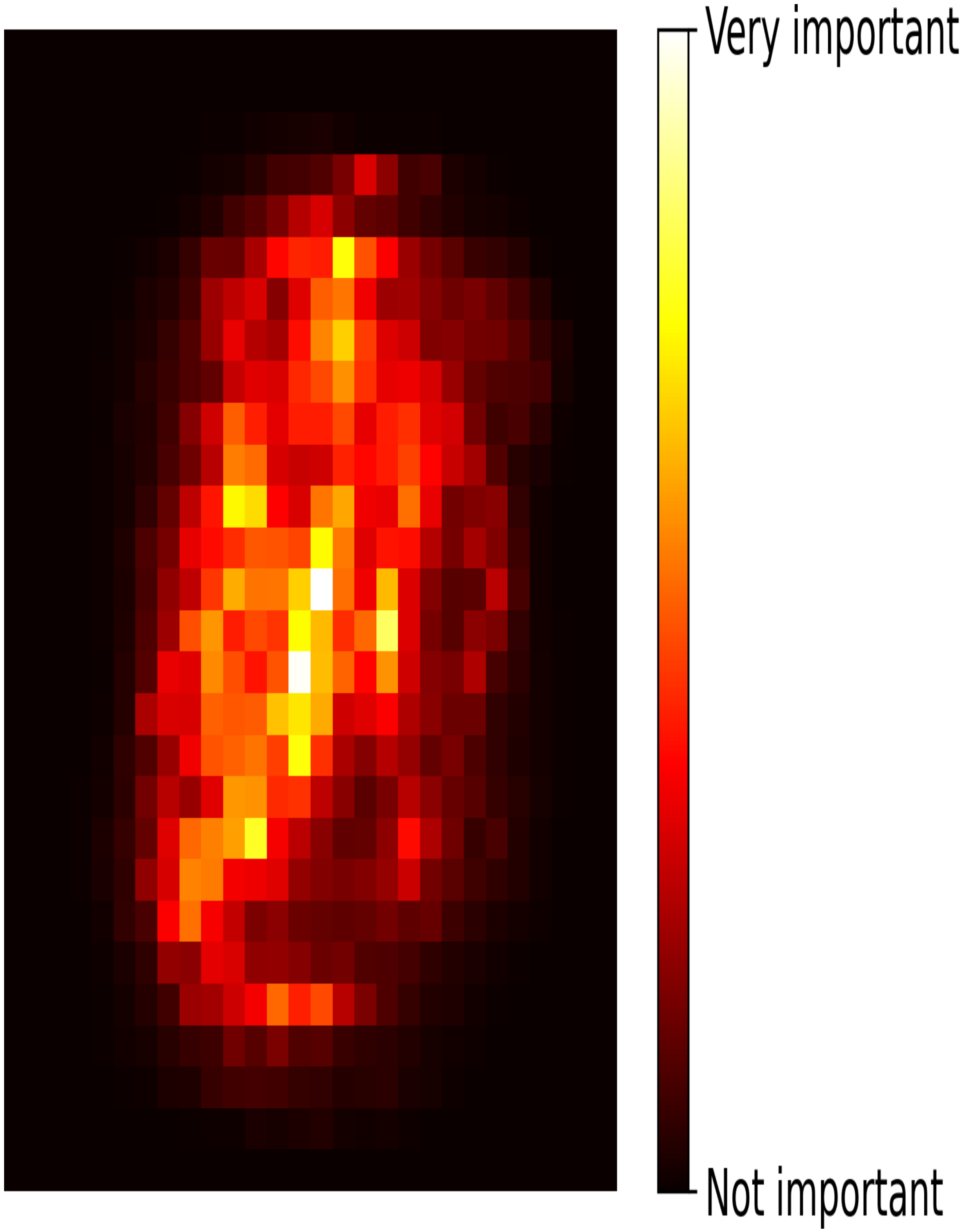


Figure 7-6. MNIST pixel importance (according to a Random Forest classifier)

Random Forests are very handy to get a quick understanding of what features actually matter, in particular if you need to perform feature selection.

Boosting

Boosting (originally called *hypothesis boosting*) refers to any Ensemble method that can combine several weak learners into a strong learner. The general idea of most boosting methods is to train predictors sequentially, each trying to correct its predecessor. There are many boosting methods available, but by far the most popular are *AdaBoost*[12] (short for *Adaptive Boosting*) and *Gradient Boosting*. Let's start with AdaBoost.

AdaBoost

One way for a new predictor to correct its predecessor is to pay a bit more attention to the training instances that the predecessor underfitted. This results in new predictors focusing more and more on the hard cases. This is the technique used by AdaBoost.

For example, when training an AdaBoost classifier, the algorithm first trains a base classifier (such as a Decision Tree) and uses it to make predictions on the training set. The algorithm then increases the relative weight of misclassified training instances. Then it trains a second classifier, using the updated weights, and again makes predictions on the training set, updates the instance weights, and so on (see Figure 7-7).

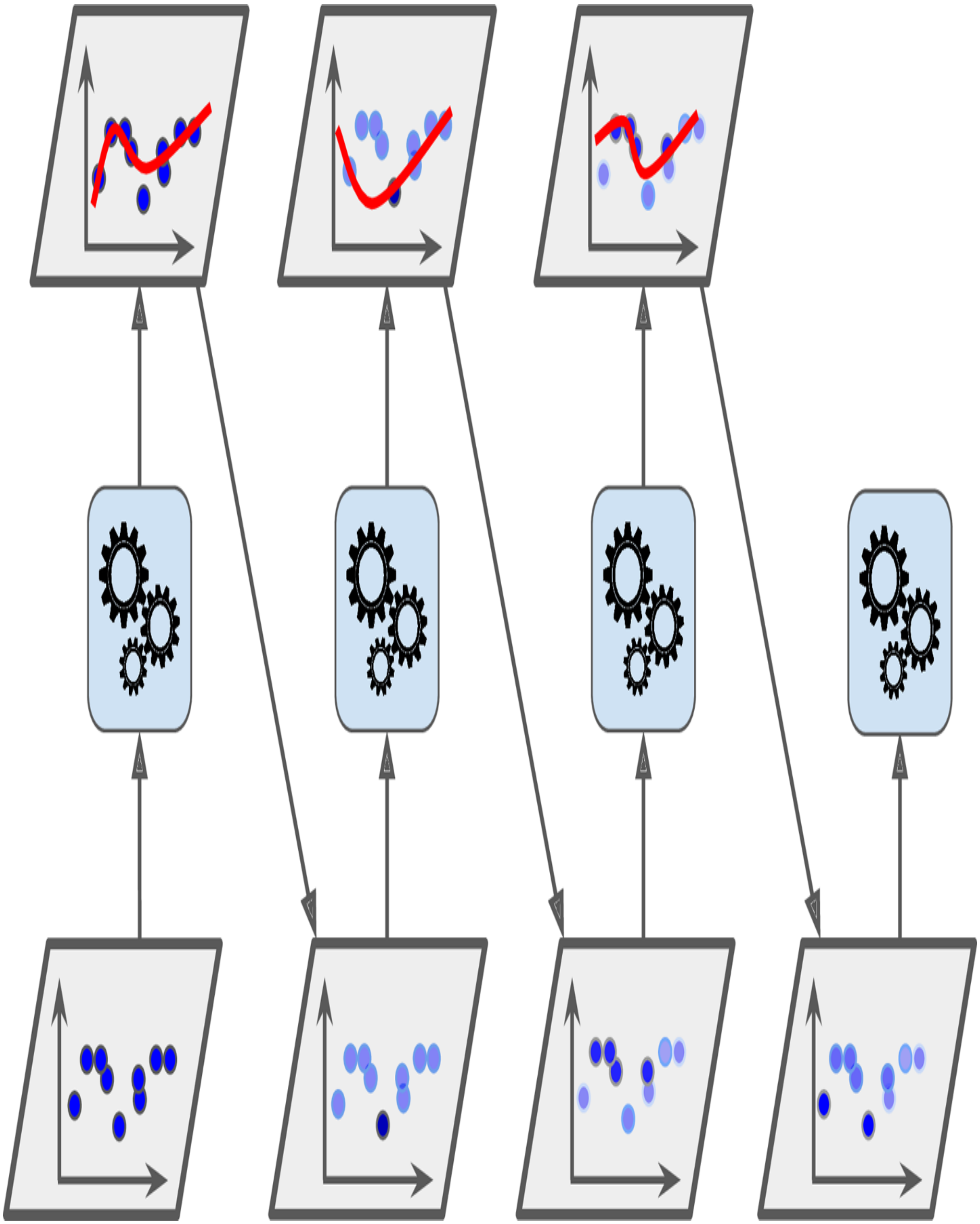


Figure 7-7. AdaBoost sequential training with instance weight updates

Figure 7-8 shows the decision boundaries of five consecutive predictors on the moons dataset (in this example, each predictor is a highly regularized SVM classifier with an RBF kernel[13]). The first classifier gets many instances wrong, so their weights get boosted. The second classifier therefore does a better job on these instances, and so on.

The plot on the right represents the same sequence of predictors, except that the learning rate is halved (i.e., the misclassified instance weights are boosted much less at every iteration). As you can see, this sequential learning technique has some similarities with Gradient Descent, except that instead of tweaking a single predictor's parameters to minimize a cost function, AdaBoost adds predictors to the ensemble, gradually making it better.

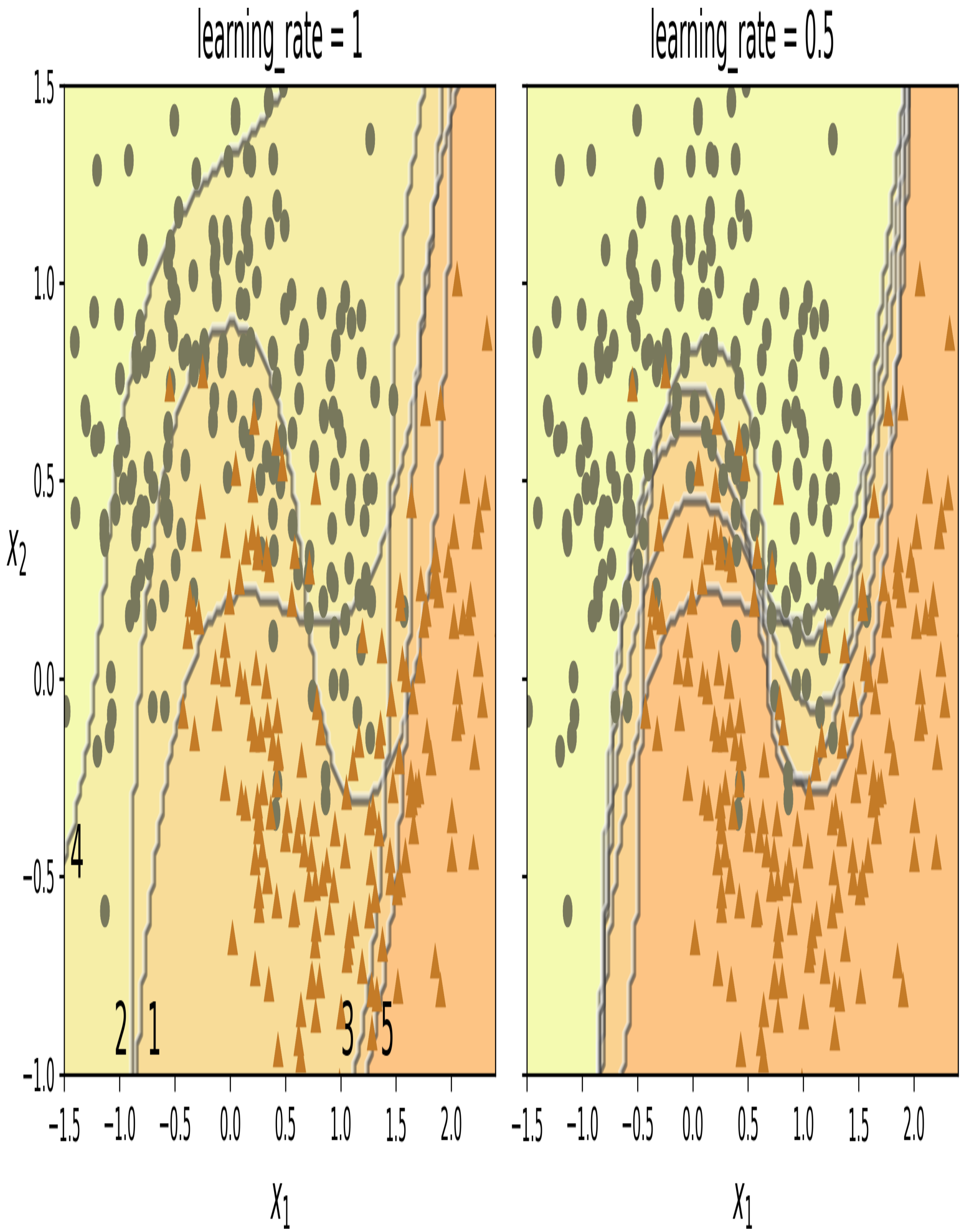


Figure 7-8. Decision boundaries of consecutive predictors

Once all predictors are trained, the ensemble makes predictions very much like bagging or pasting, except that predictors have different weights depending on their overall accuracy on the weighted training set.

> **WARNING**
>
> There is one important drawback to this sequential learning technique: training cannot be parallelized since each predictor can only be trained after the previous predictor has been trained and evaluated. As a result, it does not scale as well as bagging or pasting.

Let's take a closer look at the AdaBoost algorithm. Each instance weight $w^{(i)}$ is initially set to $1/m$. A first predictor is trained, and its weighted error rate r_1 is computed on the training set; see Equation 7-1.

Equation 7-1. Weighted error rate of the j^{th} predictor

$$r_j = \sum_{\substack{i=1 \\ \hat{y}_j^{(i)} \neq y^{(i)}}}^{m} w^{(i)} \quad \text{where } \hat{y}_j^{(i)} \text{ is the } j^{\text{th}} \text{ predictor's prediction for the } i^{\text{th}} \text{ instance.}$$

The predictor's weight α_j is then computed using Equation 7-2, where η is the learning rate hyperparameter (defaults to 1).[14] The more accurate the predictor is, the higher its weight will be. If it is just guessing randomly, then its weight will be close to zero. However, if it is most often wrong (i.e., less accurate than random guessing), then its weight will be negative.

Equation 7-2. Predictor weight

$$\alpha_j = \eta \log \frac{1 - r_j}{r_j}$$

Next, the AdaBoost algorithm updates the instance weights, using Equation 7-3, which boosts the weights of the misclassified instances.

Equation 7-3. Weight update rule

$$\begin{aligned} & \text{for } i = 1, 2, \cdots, m \\ & w^{(i)} \leftarrow \begin{cases} w^{(i)} & \text{if } \widehat{y_j}^{(i)} = y^{(i)} \\ w^{(i)} \exp\left(\alpha_j\right) & \text{if } \widehat{y_j}^{(i)} \neq y^{(i)} \end{cases} \end{aligned}$$

Then all the instance weights are normalized (i.e., divided by $\sum_{i=1}^{m} w^{(i)}$).

Finally, a new predictor is trained using the updated weights, and the whole process is repeated: the new predictor's weight is computed, the instance weights are updated, then another predictor is trained, and so on. The algorithm stops when the desired number of predictors is reached, or when a perfect predictor is found.

To make predictions, AdaBoost simply computes the predictions of all the predictors and weighs them using the predictor weights α_j. The predicted class is the one that receives the majority of weighted votes (see Equation 7-4).

Equation 7-4. AdaBoost predictions

$$\hat{y}(\mathbf{x}) = \underset{k}{\operatorname{argmax}} \sum_{\substack{j=1 \\ \hat{y}_j(\mathbf{x})=k}}^{N} \alpha_j \quad \text{where } N \text{ is the number of predictors.}$$

Scikit-Learn uses a multiclass version of AdaBoost called *SAMME*[15] (which stands for *Stagewise Additive Modeling using a Multiclass Exponential loss function*). When there are just two classes, SAMME is equivalent to AdaBoost. If the predictors can estimate class probabilities (i.e., if they have a `predict_proba()` method), Scikit-Learn can use a variant of SAMME called *SAMME.R* (the *R* stands for "Real"), which relies on class probabilities rather than predictions and generally performs better.

The following code trains an AdaBoost classifier based on 30 *Decision Stumps* using Scikit-Learn's `AdaBoostClassifier` class (as you might expect, there is also an `AdaBoostRegressor` class). A Decision Stump is a Decision Tree with `max_depth=1`—in other words, a tree composed of a single decision node plus two leaf nodes. This is the default base estimator for the `AdaBoostClassifier` class:

```
from sklearn.ensemble import AdaBoostClassifier

ada_clf = AdaBoostClassifier(
    DecisionTreeClassifier(max_depth=1), n_estimators=30,
    learning_rate=0.5, random_state=42)
ada_clf.fit(X_train, y_train)
```

> **TIP**
>
> If your AdaBoost ensemble is overfitting the training set, you can try reducing the number of estimators or more strongly regularizing the base estimator.

Gradient Boosting

Another very popular boosting algorithm is *Gradient Boosting*.[16] Just like AdaBoost, Gradient Boosting works by sequentially adding predictors to an ensemble, each one correcting its predecessor. However, instead of tweaking the instance weights at every iteration like AdaBoost does, this method tries to fit the new predictor to the *residual errors* made by the previous predictor.

Let's go through a simple regression example, using Decision Trees as the base predictors: this is called *Gradient Tree Boosting*, or *Gradient Boosted Regression Trees* (GBRT). First, let's generate a noisy quadratic dataset and fit a `DecisionTreeRegressor` to it:

```
import numpy as np
from sklearn.tree import DecisionTreeRegressor

np.random.seed(42)
X = np.random.rand(100, 1) - 0.5
y = 3 * X[:, 0] ** 2 + 0.05 * np.random.randn(100)  # y = 3x² + Gaussian
noise

tree_reg1 = DecisionTreeRegressor(max_depth=2, random_state=42)
tree_reg1.fit(X, y)
```

Next, we'll train a second `DecisionTreeRegressor` on the residual errors made by the first predictor:

```
y2 = y - tree_reg1.predict(X)
tree_reg2 = DecisionTreeRegressor(max_depth=2, random_state=43)
tree_reg2.fit(X, y2)
```

Then we train a third regressor on the residual errors made by the second predictor:

```
y3 = y2 - tree_reg2.predict(X)
tree_reg3 = DecisionTreeRegressor(max_depth=2, random_state=44)
tree_reg3.fit(X, y3)
```

Now we have an ensemble containing three trees. It can make predictions on a new instance simply by adding up the predictions of all the trees:

```
>>> X_new = np.array([[-0.4], [0.], [0.5]])
>>> sum(tree.predict(X_new) for tree in (tree_reg1, tree_reg2, tree_reg3))
array([0.49484029, 0.04021166, 0.75026781])
```

Figure 7-9 represents the predictions of these three trees in the left column, and the ensemble's predictions in the right column. In the first row, the ensemble has just one tree, so its predictions are exactly the same as the first tree's predictions. In the second row, a new tree is trained on the residual errors of the first tree. On the right you can see that the ensemble's predictions are equal to the sum of the predictions of the first two trees. Similarly, in the third row another tree is trained on the residual errors of the second tree. You can see that the ensemble's predictions gradually get better as trees are added to the ensemble.

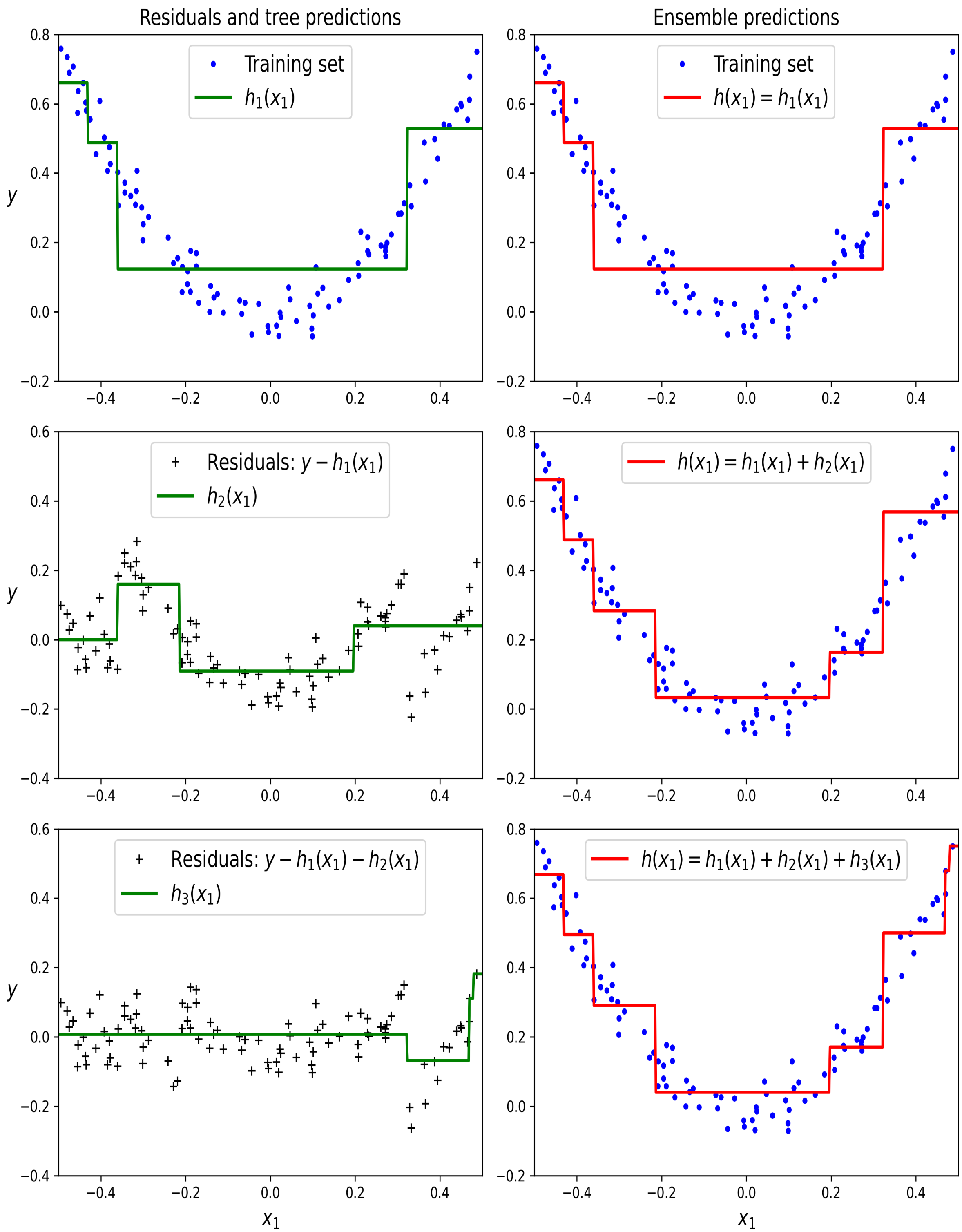


Figure 7-9. In this depiction of Gradient Boosting, the first predictor (top left) is trained normally, then each consecutive predictor (middle left and lower left) is trained on the previous predictor's residuals; the right column shows the resulting ensemble's predictions

A simpler way to train GBRT ensembles is to use Scikit-Learn's `GradientBoostingRegressor` class (there's also a

GradientBoostingClassifier class for classification). Much like the RandomForestRegressor class, it has hyperparameters to control the growth of Decision Trees (e.g., max_depth, min_samples_leaf), as well as hyperparameters to control the ensemble training, such as the number of trees (n_estimators). The following code creates the same ensemble as the previous one:

```
from sklearn.ensemble import GradientBoostingRegressor

gbrt = GradientBoostingRegressor(max_depth=2, n_estimators=3,
                                 learning_rate=1.0, random_state=42)
gbrt.fit(X, y)
```

The learning_rate hyperparameter scales the contribution of each tree. If you set it to a low value, such as 0.05, you will need more trees in the ensemble to fit the training set, but the predictions will usually generalize better. This is a regularization technique called *shrinkage*. Figure 7-10 shows two GBRT ensembles trained with different hyperparameters: the one on the left does not have enough trees to fit the training set, while the one on the right has about the right amount. If we added more, the GBRT would start to overfit the training set.

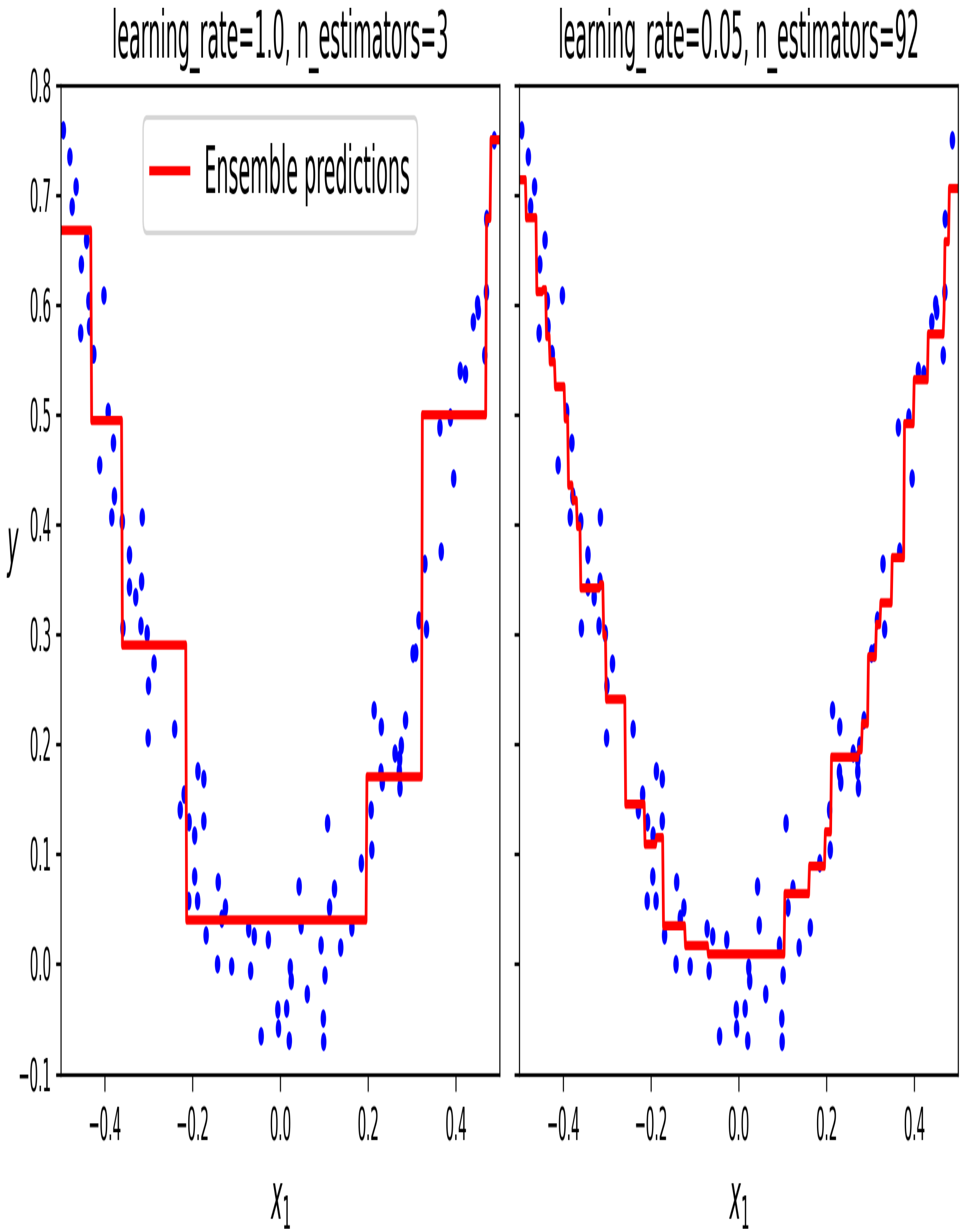


Figure 7-10. GBRT ensembles with not enough predictors (left) and just enough (right)

To find the optimal number of trees, you could perform cross-validation using `GridSearchCV` or `RandomizedSearchCV`, as usual, but there's a simpler way: if you set the `n_iter_no_change` hyperparameter to an integer value, say 10, then the

`GradientBoostingRegressor` will automatically stop adding more trees during training if it sees that the last 10 trees didn't help. This is simply early stopping (introduced in Chapter 4), but with a little bit of patience: it tolerates having no progress for a few iterations before it stops. Let's train the ensemble using early stopping:

```
gbrt_best = GradientBoostingRegressor(
    max_depth=2, learning_rate=0.05, n_estimators=500,
    n_iter_no_change=10, random_state=42)
gbrt_best.fit(X, y)
```

If you set `n_iter_no_change` too low, training may stop too early and the model will underfit. But if you set it too high, it will overfit instead. We also set a fairly small learning rate and a high number of estimators, but the actual number of estimators in the trained ensemble is much lower, thanks to early stopping:

```
>>> gbrt_best.n_estimators_
92
```

When `n_iter_no_change` is set, the `fit()` method automatically splits the training set into a smaller training set and a validation set: this allows it to evaluate the model's performance each time it adds a new tree. The size of the validation set is controlled by the `validation_fraction` hyperparameter, which is 10% by default. The `tol` hyperparameter determines the maximum performance improvement that still counts as negligible. It defaults to 0.0001.

The `GradientBoostingRegressor` class also supports a `subsample` hyperparameter, which specifies the fraction of training instances to be used for training each tree. For example, if `subsample=0.25`, then each tree is trained on 25% of the training instances, selected randomly. As you can probably guess by now, this technique trades a higher bias for a lower variance. It also speeds up training considerably. This is called *Stochastic Gradient Boosting*.

Histogram-Based Gradient Boosting

Scikit-Learn also provides another GBRT implementation, optimized for large datasets: *Histogram-based Gradient Boosting* (HGB). It works by binning the inputs features, replacing them with integers. The number of bins is controlled by the `max_bins` hyperparameter, which defaults to 255 and cannot be set any higher than this. Binning can enormously reduce the number of possible thresholds that the training algorithm needs to evaluate. Moreover, working with integers makes it possible to use faster and more memory-efficient data structures. And the way the bins are built removes the need for sorting the features when training each tree.

As a result, this implementation has a computational complexity of پ□n_×m) instead of پ□n_×m×log(m)), where m is the number of training instances, and n is the number of features. In practice, this means that HGB can train hundreds of times faster than regular GBRT on large datasets. However, binning causes a precision loss, which acts as a regularizer: depending on the dataset, this may help reduce overfitting, or it may cause underfitting.

Scikit-Learn provides two classes for HGB: `HistGradientBoostingRegressor` and `HistGradientBoostingClassifier`. They have a similar API as `GradientBoostingRegressor` and `GradientBoostingClassifier`, with a few notable differences:

- Early stopping is automatically activated if the number of instances is greater than 10,000. You can turn early-stopping always on or off by setting the `early_stopping` hyperparameter to `True` or `False`.
- Subsampling is not supported.
- `n_estimators` is renamed to `max_iter`.
- The only Decision Tree hyperparameters that can be tweaked are `max_leaf_nodes`, `min_samples_leaf`, and `max_depth`.

The HGB classes also have two nice features: they support both categorical features and missing values. This simplifies preprocessing quite a bit. However, the categorical features must be represented as integers ranging from 0 to a number lower than `max_bins`: you can use an `OrdinalEncoder` for this. For example, here's how to build and train a complete pipeline for the California housing dataset introduced in Chapter 2:

```
from sklearn.pipeline import make_pipeline
from sklearn.compose import make_column_transformer
from sklearn.ensemble import HistGradientBoostingRegressor
from sklearn.preprocessing import OrdinalEncoder

hgb_reg = make_pipeline(
    make_column_transformer((OrdinalEncoder(), ["ocean_proximity"]),
                            remainder="passthrough"),
    HistGradientBoostingRegressor(categorical_features=[0], random_state=42)
)
hgb_reg.fit(housing, housing_labels)
```

The whole pipeline is just as short as the imports! No need for an imputer, or a scaler, or a one-hot encoder, it's really convenient. Note that `categorical_features` must be set to the categorical column indices (or a boolean array). Without any hyperparameter tuning, this model yields an RMSE of about 47,600, which is not too bad.

> **TIP**
>
> Several other optimized implementations of Gradient Boosting are available in the Python ML ecosystem, in particular: XGBoost, CatBoost, and LightGBM. These libraries have been around for several years, they are all specialized for Gradient Boosting, their APIs are very similar to Scikit-Learn's, and they provide many additional features, including GPU-acceleration: you should definitely check them out! Moreover, there's a newcomer in the forest arena: TensorFlow Random Forests was released in 2021, and it provides optimized implementations of many Random Forest algorithms: plain Random Forests, Extra Trees, GBRT, and several more.

Stacking

The last Ensemble method we will discuss in this chapter is called *stacking* (short for *stacked generalization*).[17] It is based on a simple idea: instead of using trivial functions (such as hard voting) to aggregate the predictions of all predictors in an ensemble, why don't we train a model to perform this aggregation? Figure 7-11 shows such an ensemble performing a regression task on a new instance. Each of the bottom three predictors predicts a different value (3.1, 2.7, and 2.9), and then the final predictor (called a *blender*, or a *meta learner*) takes these predictions as inputs and makes the final prediction (3.0).

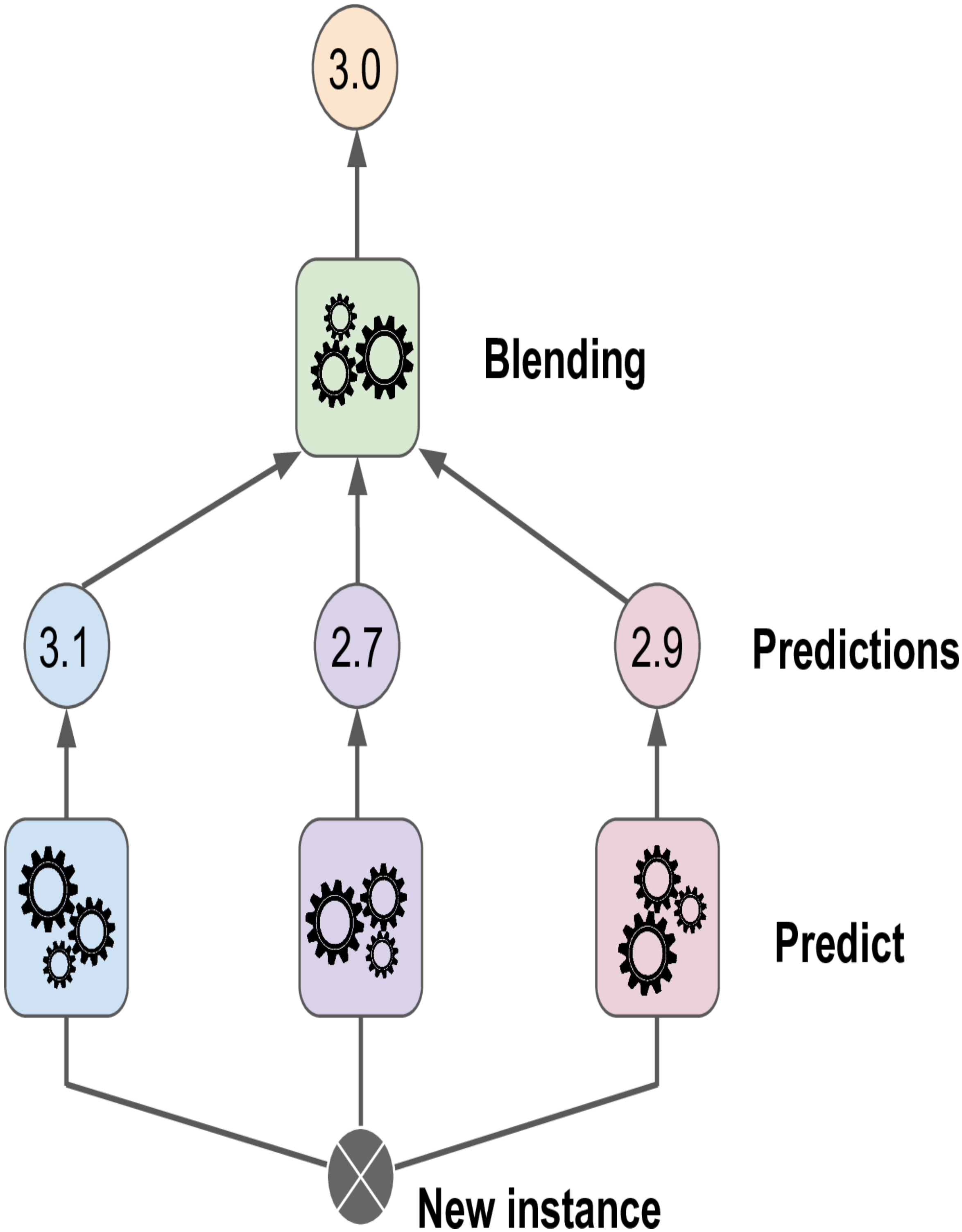


Figure 7-11. Aggregating predictions using a blending predictor

To train the blender, you first need to build the blending training set: you can use `cross_val_predict()` on every predictor in the ensemble to get out-of-sample predictions for each instance in the original training set (Figure 7-12). These can be used as the input features to train the blender, and the targets can be simply be copied from the original training set. Note that regardless of the number of features in the original training set (just one in this example), the blending training set will contain one input feature per predictor (three in this example). Once the blender is trained, the base predictors are retrained one last time on the full original training set.

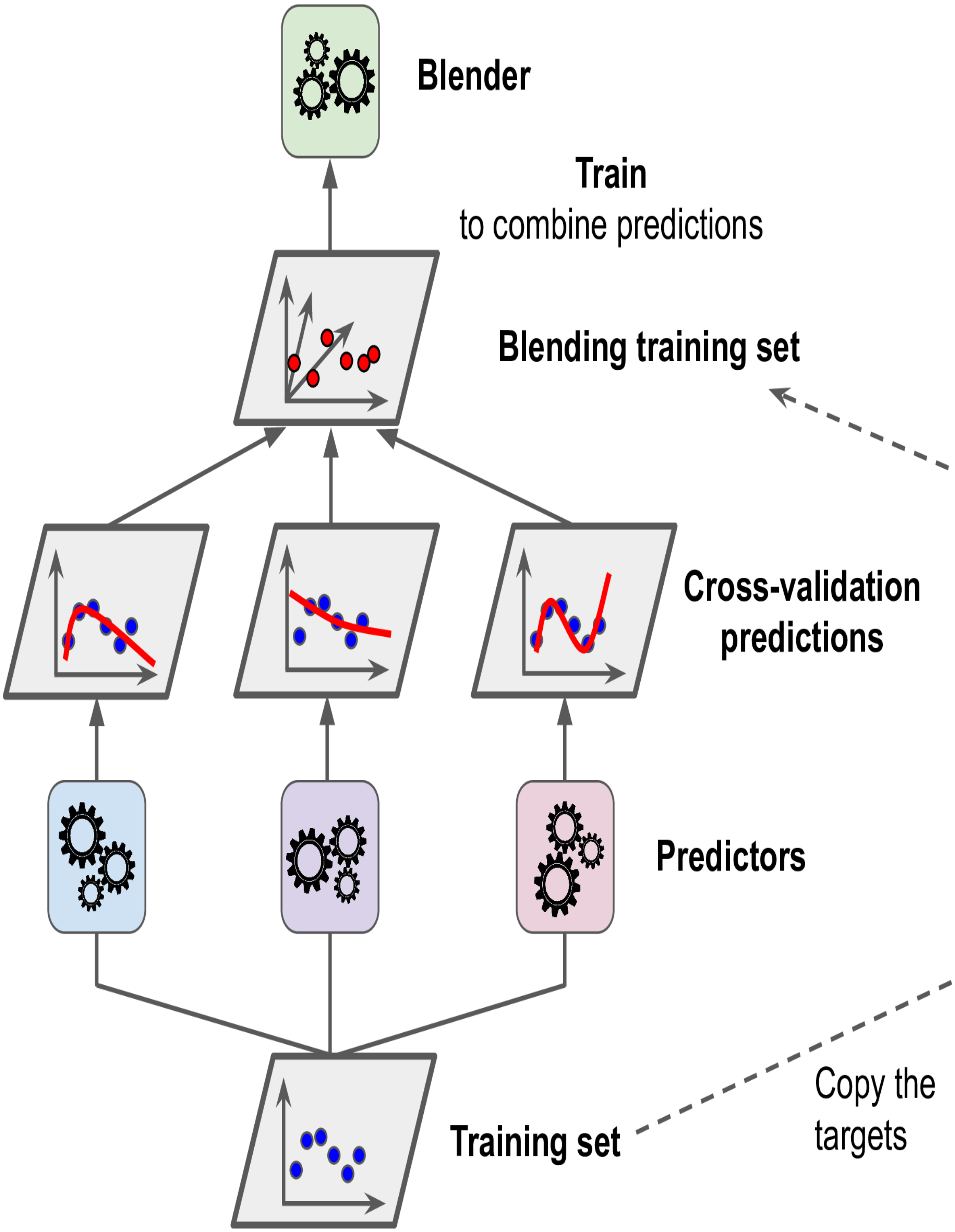


Figure 7-12. Training the blender in a stacking ensemble

It is actually possible to train several different blenders this way (e.g., one using Linear Regression, another using Random Forest Regression), to get a whole layer of blenders, and then add another blender on top of that to produce the final prediction, as shown in

Figure 7-13. You may be able to squeeze out a few more drops of performance doing this, but it will cost you in both training time and system complexity.

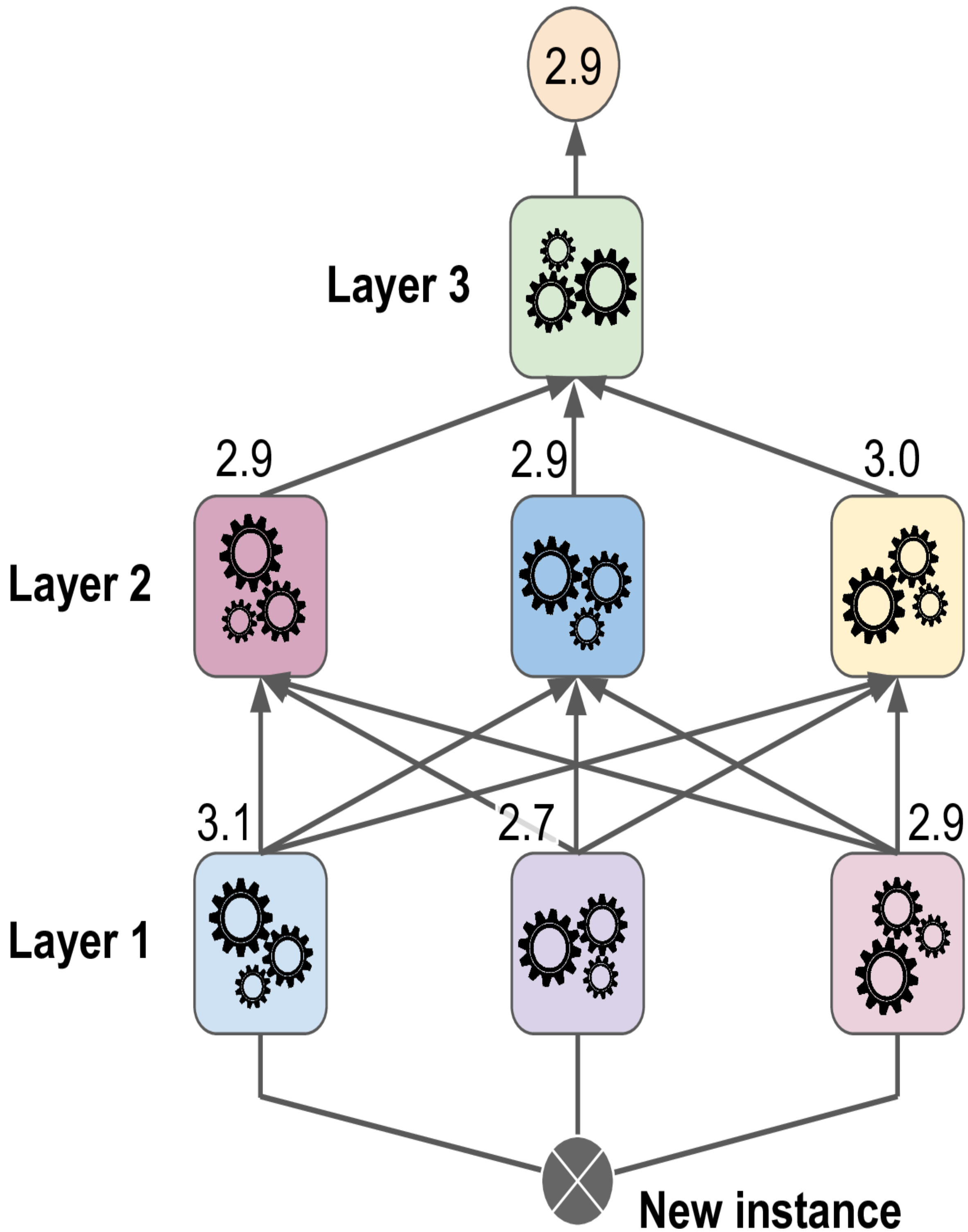


Figure 7-13. Predictions in a multilayer stacking ensemble

Scikit-Learn provides two classes for stacking ensembles: StackingClassifier and StackingRegressor. For example, you can replace the VotingClassifier you used at the beginning of this chapter on the moons dataset with a StackingClassifier:

```
from sklearn.ensemble import StackingClassifier

stacking_clf = StackingClassifier(
    estimators=[
        ('lr', LogisticRegression(random_state=42)),
        ('rf', RandomForestClassifier(random_state=42)),
        ('svc', SVC(probability=True, random_state=42))
    ],
    final_estimator=RandomForestClassifier(random_state=43),
    cv=5  # number of cross-validation folds
)
stacking_clf.fit(X_train, y_train)
```

For each predictor, the stacking classifier will call predict_proba() if available, or it will fallback to decision_function() if available, or as a last resort it will call predict(). If you don't provide a final estimator, StackingClassifier will use LogisticRegression, and StackingRegressor will use RidgeCV.

If you evaluate this stacking model on the test set, you will find 92.8% accuracy, which is a bit better than the voting classifier using soft voting, which got 92%.

In conclusion, ensemble learning is versatile, powerful, and fairly simple to use. Random Forests, AdaBoost and GBRT are among the first models you should test on most Machine Learning tasks, and they particularly shine with heterogeneous tabular data. Moreover, as they require very little preprocessing, they're great to get a prototype up and running quickly. Lastly, ensemble methods like voting classifiers and stacking classifiers can help push your system's performance to its limits.

Exercises

1. If you have trained five different models on the exact same training data, and they all achieve 95% precision, is there any chance that you can combine these models to get better results? If so, how? If not, why?
2. What is the difference between hard and soft voting classifiers?
3. Is it possible to speed up training of a bagging ensemble by distributing it across multiple servers? What about pasting ensembles, boosting ensembles, Random Forests, or stacking ensembles?

4. What is the benefit of out-of-bag evaluation?

5. What makes Extra-Trees more random than regular Random Forests? How can this extra randomness help? Are Extra-Trees slower or faster than regular Random Forests?

6. If your AdaBoost ensemble underfits the training data, which hyperparameters should you tweak and how?

7. If your Gradient Boosting ensemble overfits the training set, should you increase or decrease the learning rate?

8. Load the MNIST data (introduced in Chapter 3), and split it into a training set, a validation set, and a test set (e.g., use 50,000 instances for training, 10,000 for validation, and 10,000 for testing). Then train various classifiers, such as a Random Forest classifier, an Extra-Trees classifier, and an SVM classifier. Next, try to combine them into an ensemble that outperforms each individual classifier on the validation set, using soft or hard voting. Once you have found one, try it on the test set. How much better does it perform compared to the individual classifiers?

9. Run the individual classifiers from the previous exercise to make predictions on the validation set, and create a new training set with the resulting predictions: each training instance is a vector containing the set of predictions from all your classifiers for an image, and the target is the image's class. Train a classifier on this new training set. Congratulations, you have just trained a blender, and together with the classifiers it forms a stacking ensemble! Now evaluate the ensemble on the test set. For each image in the test set, make predictions with all your classifiers, then feed the predictions to the blender to get the ensemble's predictions. How does it compare to the voting classifier you trained earlier? Now try again using a `StackingClassifier` instead: do you get better performance? If so, why?

Solutions to these exercises are available at the end of this chapter's notebook, at *https://homl.info/colab3*.

---

1 Leo Breiman, "Bagging Predictors," *Machine Learning* 24, no. 2 (1996): 123–140.

2 In statistics, resampling with replacement is called *bootstrapping*.

3 Leo Breiman, "Pasting Small Votes for Classification in Large Databases and On-Line," *Machine Learning* 36, no. 1–2 (1999): 85–103.

4 Bias and variance were introduced in Chapter 4.

5 `max_samples` can alternatively be set to a float between 0.0 and 1.0, in which case the max number of sampled instances is equal to the size of the training set times `max_samples`.

6 As *m* grows, this ratio approaches 1 – exp(–1) ≈ 63%.

7 Gilles Louppe and Pierre Geurts, "Ensembles on Random Patches," *Lecture Notes in Computer Science* 7523 (2012): 346–361.

8 Tin Kam Ho, "The Random Subspace Method for Constructing Decision Forests," *IEEE Transactions on Pattern Analysis and Machine Intelligence* 20, no. 8 (1998): 832–844.

9 Tin Kam Ho, "Random Decision Forests," *Proceedings of the Third International Conference on Document Analysis and Recognition* 1 (1995): 278.

10 The `BaggingClassifier` class remains useful if you want a bag of something other than Decision Trees.

11 Pierre Geurts et al., "Extremely Randomized Trees," *Machine Learning* 63, no. 1 (2006): 3–42.

12 Yoav Freund and Robert E. Schapire, "A Decision-Theoretic Generalization of On-Line Learning and an Application to Boosting," *Journal of Computer and System Sciences* 55, no. 1 (1997): 119–139.

13 This is just for illustrative purposes. SVMs are generally not good base predictors for AdaBoost; they are slow and tend to be unstable with it.

14 The original AdaBoost algorithm does not use a learning rate hyperparameter.

15 For more details, see Ji Zhu et al., "Multi-Class AdaBoost," *Statistics and Its Interface* 2, no. 3 (2009): 349–360.

16 Gradient Boosting was first introduced in Leo Breiman's 1997 paper "Arcing the Edge" and was further developed in the 1999 paper "Greedy Function Approximation: A Gradient Boosting Machine" by Jerome H. Friedman.

17 David H. Wolpert, "Stacked Generalization," *Neural Networks* 5, no. 2 (1992): 241–259.

Chapter 8. Dimensionality Reduction

A NOTE FOR EARLY RELEASE READERS

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.

This will be the 8th chapter of the final book. Notebooks are available on GitHub at *https://github.com/ageron/handson-ml3*. Datasets are available at *https://github.com/ageron/data*.

If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the editoor at ntache@oreilly.com.

Many Machine Learning problems involve thousands or even millions of features for each training instance. Not only do all these features make training extremely slow, but they can also make it much harder to find a good solution, as we will see. This problem is often referred to as the *curse of dimensionality*.

Fortunately, in real-world problems, it is often possible to reduce the number of features considerably, turning an intractable problem into a tractable one. For example, consider the MNIST images (introduced in Chapter 3): the pixels on the image borders are almost always white, so you could completely drop these pixels from the training set without losing much information. Figure 7-6 confirms that these pixels are utterly unimportant for the classification task. Additionally, two neighboring pixels are often highly correlated: if you merge them into a single pixel (e.g., by taking the mean of the two pixel intensities), you will not lose much information.

> **WARNING**
>
> Reducing dimensionality does cause some information loss, just like compressing an image to JPEG can degrade its quality, so even though it will speed up training, it may make your system perform slightly worse. It also makes your pipelines a bit more complex and thus harder to maintain. So you should first try to train your system with the original data before considering using dimensionality reduction. In some cases, reducing the dimensionality of the training data may filter out some noise and unnecessary details and thus result in higher performance, but in general it won't; it will just speed up training.

Apart from speeding up training, dimensionality reduction is also extremely useful for data visualization (or *DataViz*). Reducing the number of dimensions down to two (or three) makes it possible to plot a condensed view of a high-dimensional training set on a graph and often gain some important insights by visually detecting patterns, such as clusters. Moreover, DataViz is essential to communicate your conclusions to people who are not data scientists—in particular, decision makers who will use your results.

In this chapter we will discuss the curse of dimensionality and get a sense of what goes on in high-dimensional space. Then, we will consider the two main approaches to dimensionality reduction (projection and Manifold Learning), and we will go through three of the most popular dimensionality reduction techniques: PCA, random projection, and LLE.

The Curse of Dimensionality

We are so used to living in three dimensions[1] that our intuition fails us when we try to imagine a high-dimensional space. Even a basic 4D hypercube is incredibly hard to picture in our minds (see Figure 8-1), let alone a 200-dimensional ellipsoid bent in a 1,000-dimensional space.

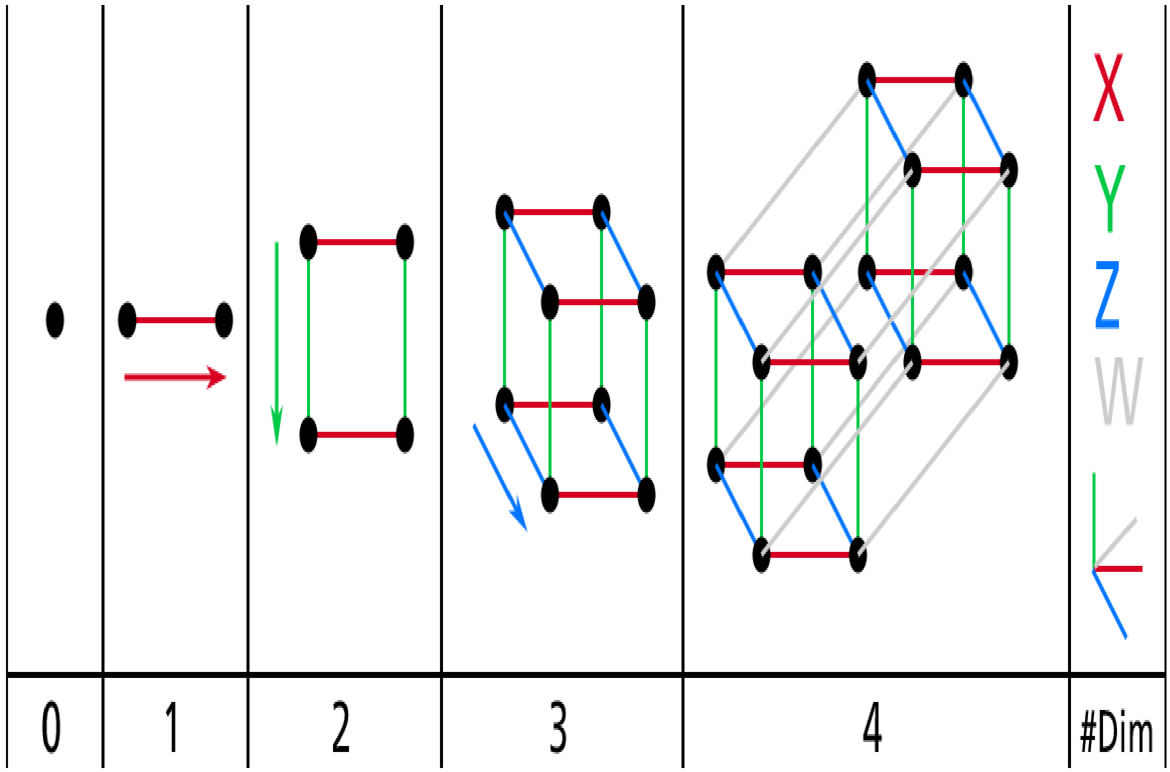


Figure 8-1. Point, segment, square, cube, and tesseract (0D to 4D hypercubes)[2]

It turns out that many things behave very differently in high-dimensional space. For example, if you pick a random point in a unit square (a 1 × 1 square), it will have only about a 0.4% chance of being located less than 0.001 from a border (in other words, it is very unlikely that a random point will be "extreme" along any dimension). But in a 10,000-dimensional unit hypercube, this probability is greater than 99.999999%. Most points in a high-dimensional hypercube are very close to the border.[3]

Here is a more troublesome difference: if you pick two points randomly in a unit square, the distance between these two points will be, on average, roughly 0.52. If you pick two random points in a unit 3D cube, the average distance will be roughly 0.66. But what about two points picked randomly in a 1,000,000-dimensional hypercube? The average distance, believe it or not, will be about 408.25 (roughly $\sqrt{1,000,000/6}$)! This is counterintuitive: how can two points be so far apart when they both lie within the same unit hypercube? Well, there's just plenty of space in high dimensions. As a result, high-dimensional datasets are at risk of being very sparse: most training instances are likely to be far away from each other. This also means that a new instance will likely be far away from any training instance, making predictions much less reliable than in lower dimensions, since they will be based on much larger extrapolations. In short, the more dimensions the training set has, the greater the risk of overfitting it.

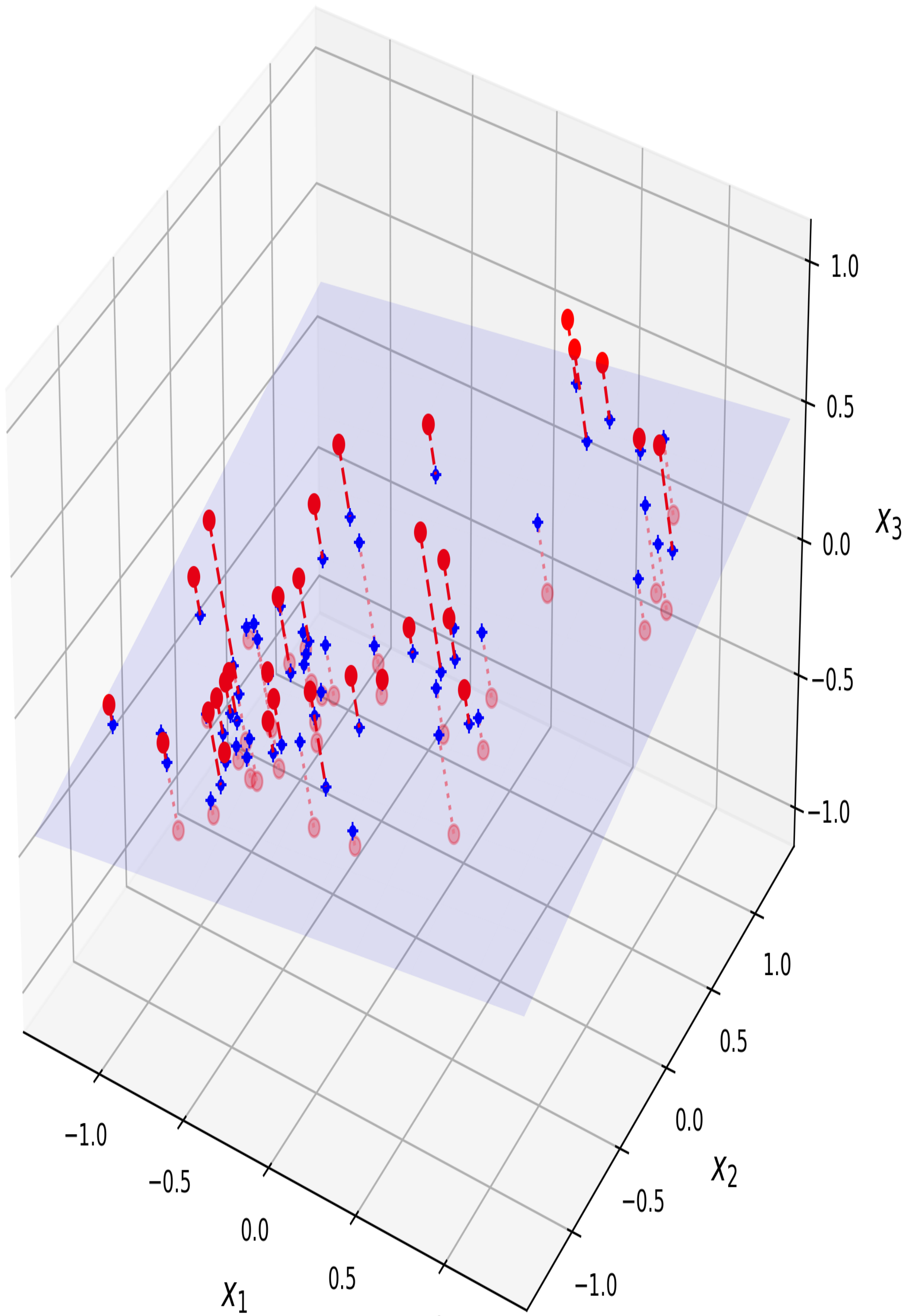
In theory, one solution to the curse of dimensionality could be to increase the size of the training set to reach a sufficient density of training instances. Unfortunately, in practice, the number of training instances required to reach a given density grows exponentially with the number of dimensions. With just 100 features—significantly fewer than in the MNIST problem—all ranging from 0 to 1, you would need more training instances than atoms in the observable universe in order for training instances to be within 0.1 of each other on average, assuming they were spread out uniformly across all dimensions.

Main Approaches for Dimensionality Reduction

Before we dive into specific dimensionality reduction algorithms, let's take a look at the two main approaches to reducing dimensionality: projection and Manifold Learning.

Projection

In most real-world problems, training instances are *not* spread out uniformly across all dimensions. Many features are almost constant, while others are highly correlated (as discussed earlier for MNIST). As a result, all training instances lie within (or close to) a much lower-dimensional *subspace* of the high-dimensional space. This sounds very abstract, so let's look at an example. In Figure 8-2 you can see a 3D dataset represented by small spheres.



x_1
x_2
x_3
−1.0
−0.5
0.0
0.5
1.0

Figure 8-2. A 3D dataset lying close to a 2D subspace

Notice that all training instances lie close to a plane: this is a lower-dimensional (2D) subspace of the higher-dimensional (3D) space. If we project every training instance perpendicularly onto this subspace (as represented by the short dashed lines connecting the instances to the plane), we get the new 2D dataset shown in Figure 8-3. Ta-da! We have just reduced the dataset's dimensionality from 3D to 2D. Note that the axes correspond to new features z_1 and z_2: they are the coordinates of the projections on the plane.

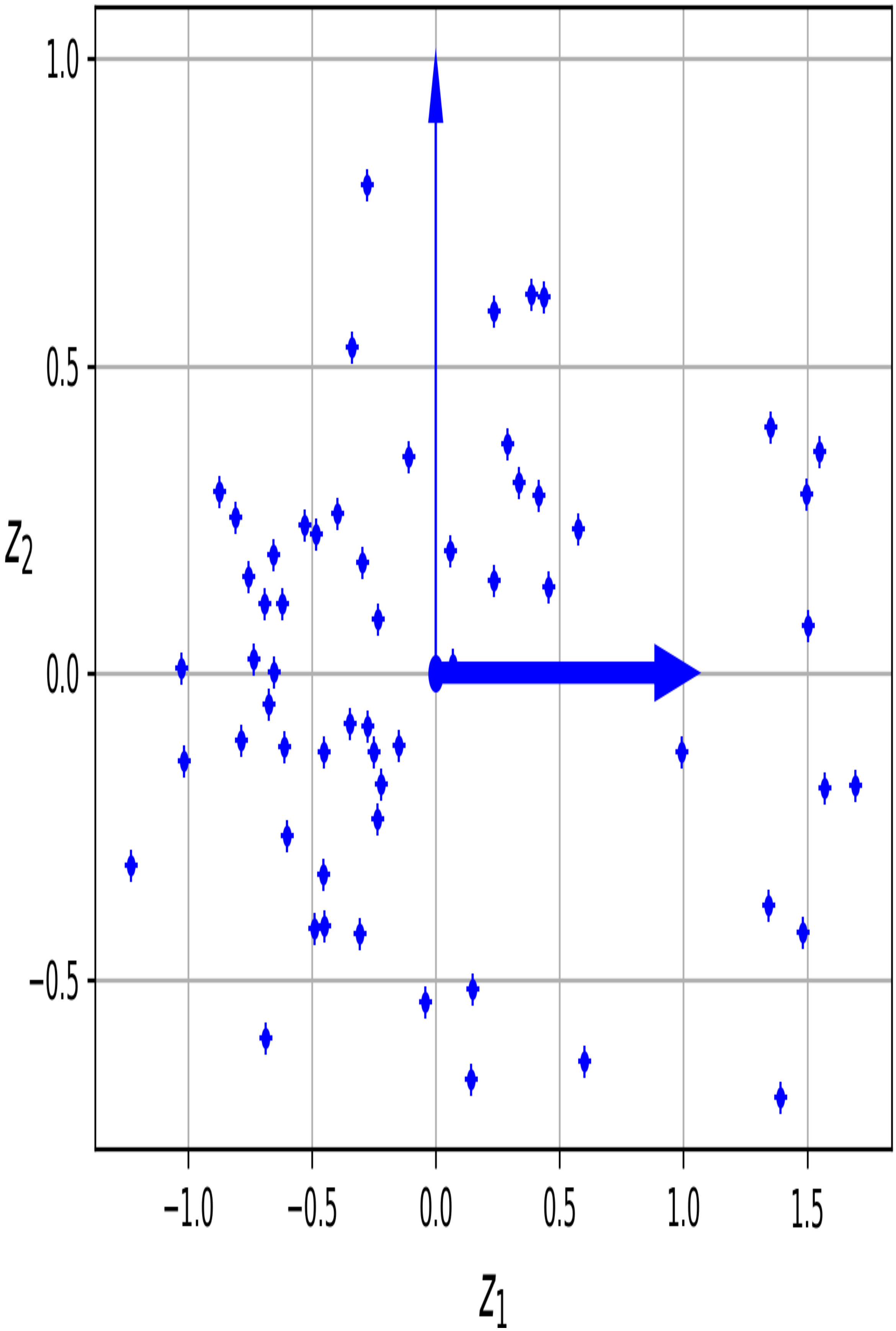

1.0
0.5
0.0
−0.5
z_2
−1.0
−0.5
0.0
0.5
1.0
1.5
z_1

Figure 8-3. The new 2D dataset after projection

However, projection is not always the best approach to dimensionality reduction. In many cases the subspace may twist and turn, such as in the famous *Swiss roll* toy dataset represented in Figure 8-4.

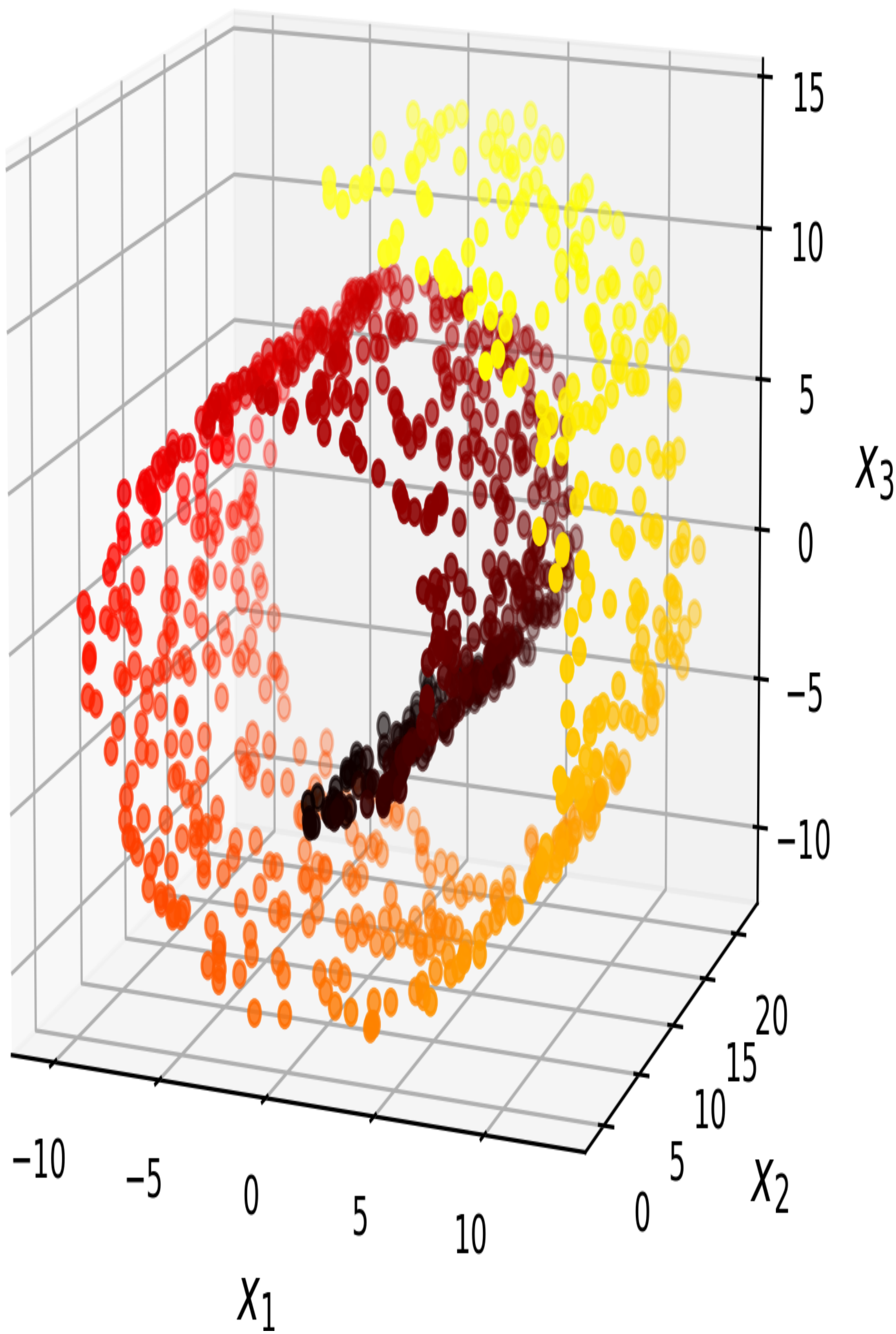
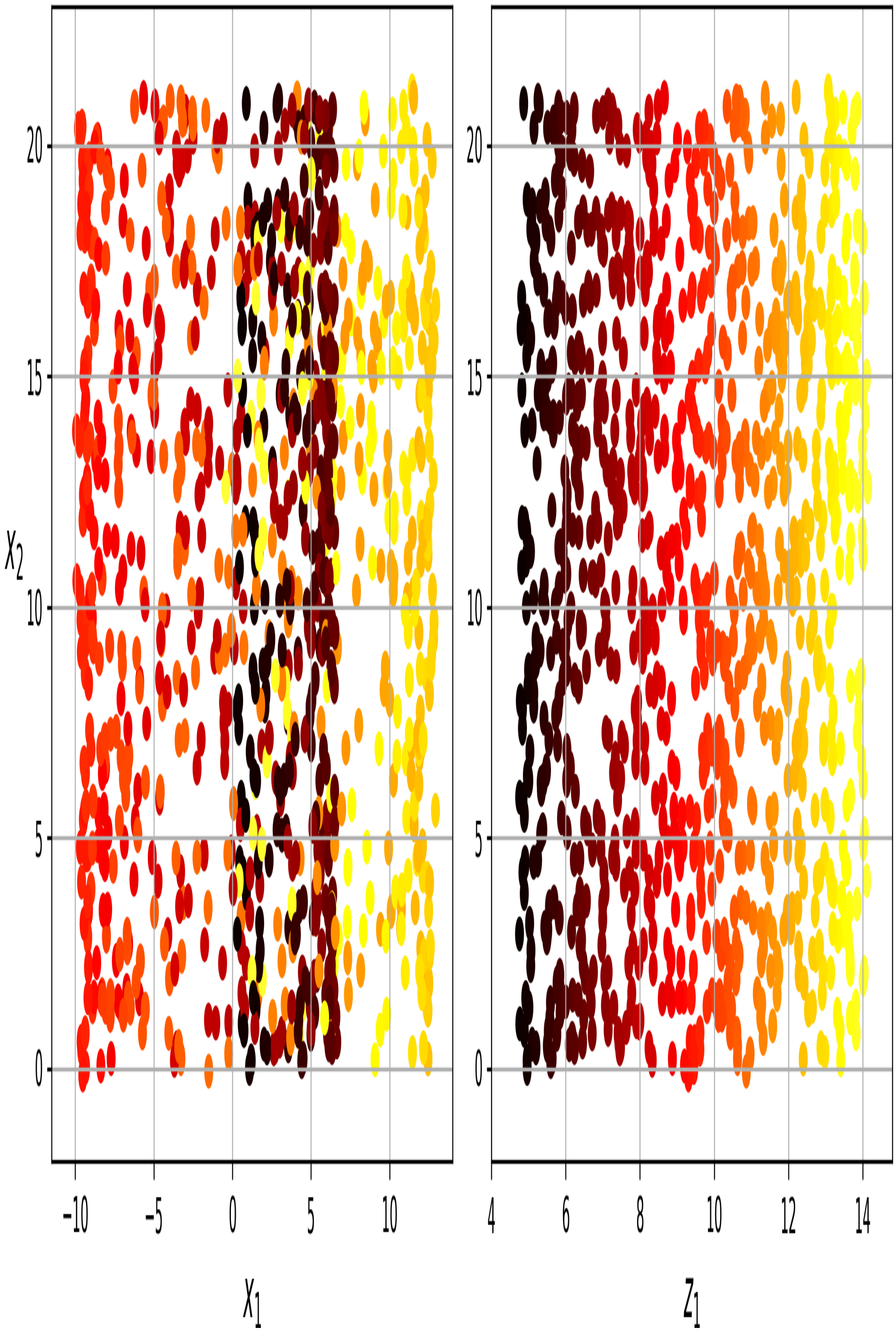

15
10
5
0
−5
−10
x_3
20
15
10
5
0
x_2
−10
−5
0
5
10
x_1

Figure 8-4. Swiss roll dataset

Simply projecting onto a plane (e.g., by dropping x_3) would squash different layers of the Swiss roll together, as shown on the left side of Figure 8-5. What you probably want instead is to unroll the Swiss roll to obtain the 2D dataset on the right side of Figure 8-5.



X_2
20
15
10
5
0
-10
-5
0
5
10
X_1
20
15
10
5
0
4
6
8
10
12
14
Z_1

Figure 8-5. Squashing by projecting onto a plane (left) versus unrolling the Swiss roll (right)

Manifold Learning

The Swiss roll is an example of a 2D *manifold*. Put simply, a 2D manifold is a 2D shape that can be bent and twisted in a higher-dimensional space. More generally, a d-dimensional manifold is a part of an n-dimensional space (where $d < n$) that locally resembles a d-dimensional hyperplane. In the case of the Swiss roll, $d = 2$ and $n = 3$: it locally resembles a 2D plane, but it is rolled in the third dimension.

Many dimensionality reduction algorithms work by modeling the manifold on which the training instances lie; this is called *Manifold Learning*. It relies on the *manifold assumption*, also called the *manifold hypothesis*, which holds that most real-world high-dimensional datasets lie close to a much lower-dimensional manifold. This assumption is very often empirically observed.

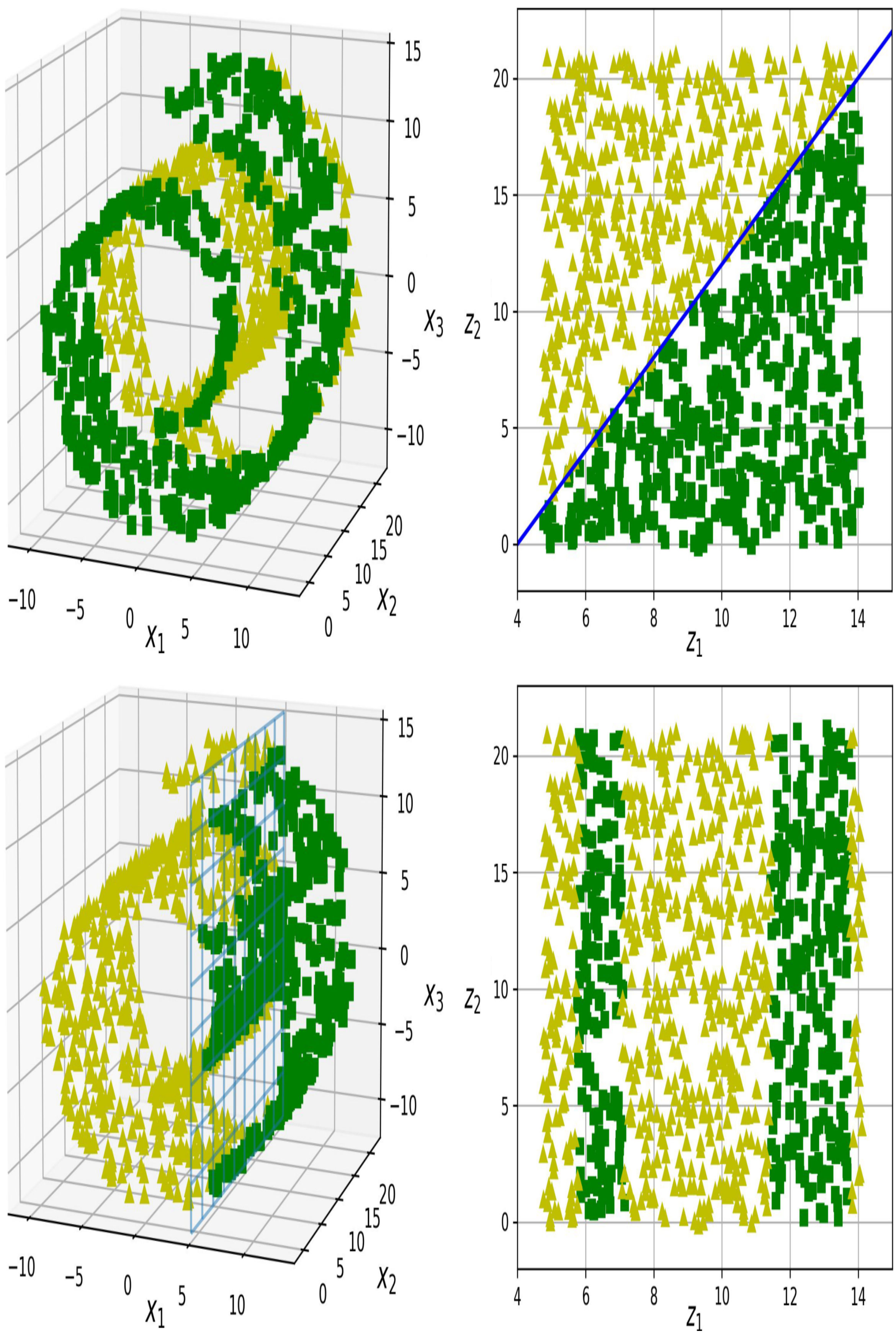
Once again, think about the MNIST dataset: all handwritten digit images have some similarities. They are made of connected lines, the borders are white, and they are more or less centered. If you randomly generated images, only a ridiculously tiny fraction of them would look like handwritten digits. In other words, the degrees of freedom available to you if you try to create a digit image are dramatically lower than the degrees of freedom you have if you are allowed to generate any image you want. These constraints tend to squeeze the dataset into a lower-dimensional manifold.

The manifold assumption is often accompanied by another implicit assumption: that the task at hand (e.g., classification or regression) will be simpler if expressed in the lower-dimensional space of the manifold. For example, in the top row of Figure 8-6 the Swiss roll is split into two classes: in the 3D space (on the left), the decision boundary would be fairly complex, but in the 2D unrolled manifold space (on the right), the decision boundary is a straight line.

However, this implicit assumption does not always hold. For example, in the bottom row of Figure 8-6, the decision boundary is located at $x_1 = 5$. This decision boundary looks very simple in the original 3D space (a vertical plane), but it looks more complex in the unrolled manifold (a collection of four independent line segments).

In short, reducing the dimensionality of your training set before training a model will usually speed up training, but it may not always lead to a better or simpler solution; it all depends on the dataset.

Hopefully you now have a good sense of what the curse of dimensionality is and how dimensionality reduction algorithms can fight it, especially when the manifold assumption holds. The rest of this chapter will go through some of the most popular algorithms.



x_1
x_2
x_3
z_1
z_2

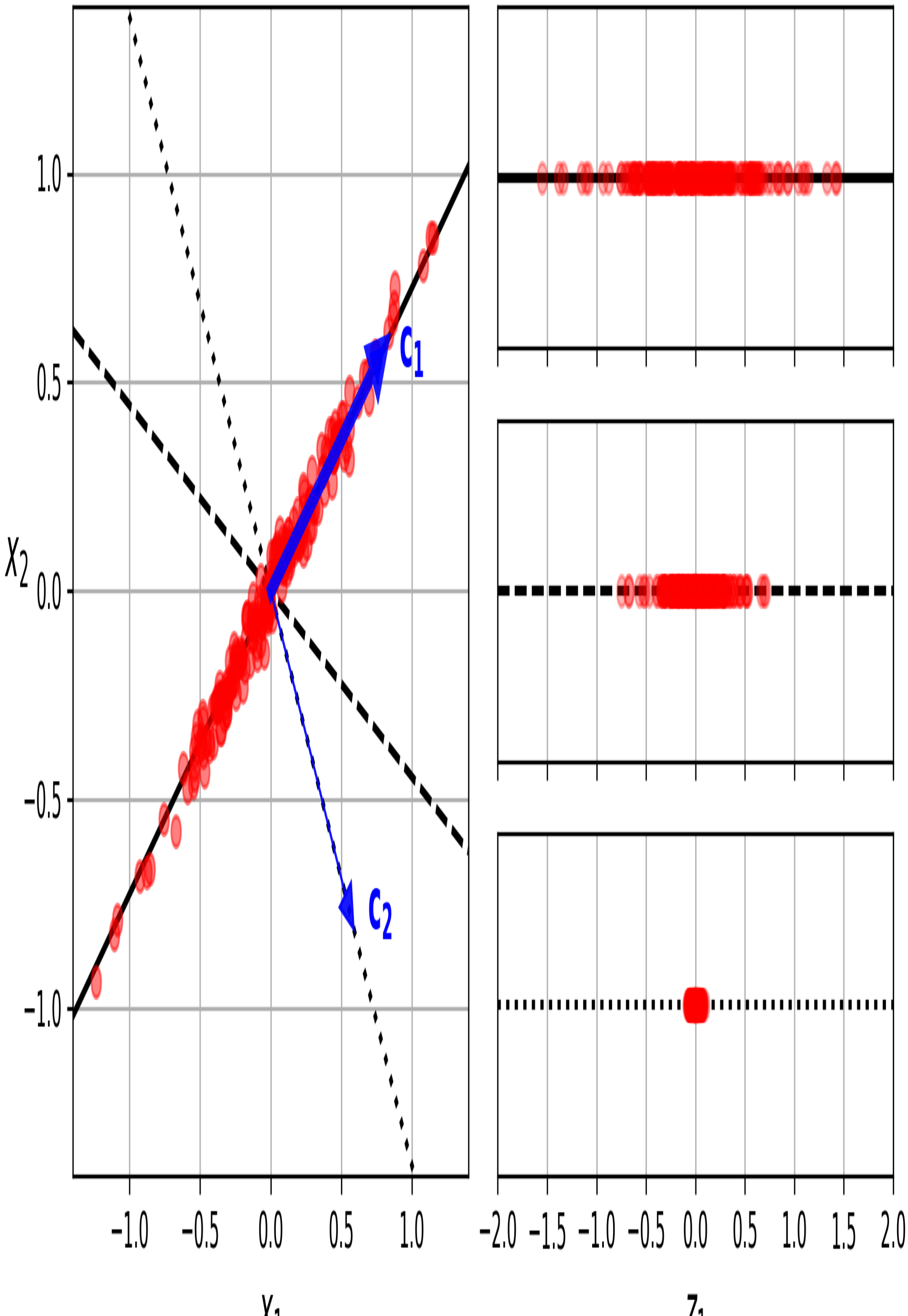
Figure 8-6. The decision boundary may not always be simpler with lower dimensions

PCA

Principal Component Analysis (PCA) is by far the most popular dimensionality reduction algorithm. First it identifies the hyperplane that lies closest to the data, and then it projects the data onto it, just like in Figure 8-2.

Preserving the Variance

Before you can project the training set onto a lower-dimensional hyperplane, you first need to choose the right hyperplane. For example, a simple 2D dataset is represented on the left in Figure 8-7, along with three different axes (i.e., 1D hyperplanes). On the right is the result of the projection of the dataset onto each of these axes. As you can see, the projection onto the solid line preserves the maximum variance, while the projection onto the dotted line preserves very little variance and the projection onto the dashed line preserves an intermediate amount of variance.



c_1
c_2
x_2
x_1
z_1

Figure 8-7. Selecting the subspace to project on

It seems reasonable to select the axis that preserves the maximum amount of variance, as it will most likely lose less information than the other projections. Another way to justify this choice is that it is the axis that minimizes the mean squared distance between the original dataset and its projection onto that axis. This is the rather simple idea behind PCA.[4]

Principal Components

PCA identifies the axis that accounts for the largest amount of variance in the training set. In Figure 8-7, it is the solid line. It also finds a second axis, orthogonal to the first one, that accounts for the largest amount of remaining variance. In this 2D example there is no choice: it is the dotted line. If it were a higher-dimensional dataset, PCA would also find a third axis, orthogonal to both previous axes, and a fourth, a fifth, and so on—as many axes as the number of dimensions in the dataset.

The i^{th} axis is called the i^{th} *principal component* (PC) of the data. In Figure 8-7, the first PC is the axis on which vector $\mathbf{c_1}$ lies, and the second PC is the axis on which vector $\mathbf{c_2}$ lies. In Figure 8-2 the first two PCs are on the projection plane, and the third PC is the axis orthogonal to that plane. After the projection, in Figure 8-3, the first PC corresponds to the z_1 axis, and the second PC corresponds to the z_2 axis.

> **NOTE**
>
> For each principal component, PCA finds a zero-centered unit vector pointing in the direction of the PC. Since two opposing unit vectors lie on the same axis, the direction of the unit vectors returned by PCA is not stable: if you perturb the training set slightly and run PCA again, the unit vectors may point in the opposite direction as the original vectors. However, they will generally still lie on the same axes. In some cases, a pair of unit vectors may even rotate or swap (if the variances along these two axes are very close), but the plane they define will generally remain the same.

So how can you find the principal components of a training set? Luckily, there is a standard matrix factorization technique called *Singular Value Decomposition* (SVD) that can decompose the training set matrix $\mathbf{X}$ into the matrix multiplication of three matrices $\mathbf{U}\ \mathbf{\Sigma}\ \mathbf{V}^\intercal$, where $\mathbf{V}$ contains the unit vectors that define all the principal components that we are looking for, as shown in Equation 8-1.

Equation 8-1. Principal components matrix

$$\mathbf{V} = \begin{pmatrix} \mid & \mid & & \mid \\ \mathbf{c}_1 & \mathbf{c}_2 & \cdots & \mathbf{c}_n \\ \mid & \mid & & \mid \end{pmatrix}$$

The following Python code uses NumPy's `svd()` function to obtain all the principal components of the 3D training set represented in Figure 8-2, then it extracts the two unit vectors that define the first two PCs:

```
import numpy as np

X = [...]  # create a small 3D dataset
X_centered = X - X.mean(axis=0)
U, s, Vt = np.linalg.svd(X_centered)
c1 = Vt[0]
c2 = Vt[1]
```

> **WARNING**
>
> PCA assumes that the dataset is centered around the origin. As we will see, Scikit-Learn's PCA classes take care of centering the data for you. If you implement PCA yourself (as in the preceding example), or if you use other libraries, don't forget to center the data first.

Projecting Down to *d* Dimensions

Once you have identified all the principal components, you can reduce the dimensionality of the dataset down to *d* dimensions by projecting it onto the hyperplane defined by the first *d* principal components. Selecting this hyperplane ensures that the projection will preserve as much variance as possible. For example, in Figure 8-2 the 3D dataset is projected down to the 2D plane defined by the first two principal components, preserving a large part of the dataset's variance. As a result, the 2D projection looks very much like the original 3D dataset.

To project the training set onto the hyperplane and obtain a reduced dataset $\mathbf{X}_{d\text{-proj}}$ of dimensionality d, compute the matrix multiplication of the training set matrix $\mathbf{X}$ by the matrix $\mathbf{W}_d$, defined as the matrix containing the first d columns of $\mathbf{V}$, as shown in Equation 8-2.

Equation 8-2. Projecting the training set down to d dimensions

$$\mathbf{X}_{d\text{-proj}} = \mathbf{X}\mathbf{W}_d$$

The following Python code projects the training set onto the plane defined by the first two principal components:

```
W2 = Vt[:2].T
X2D = X_centered @ W2
```

There you have it! You now know how to reduce the dimensionality of any dataset by projecting it down to any number of dimensions, while preserving as much variance as possible.

Using Scikit-Learn

Scikit-Learn's `PCA` class uses SVD decomposition to implement PCA, just like we did earlier in this chapter. The following code applies PCA to reduce the dimensionality of the dataset down to two dimensions (note that it automatically takes care of centering the data):

```
from sklearn.decomposition import PCA

pca = PCA(n_components=2)
X2D = pca.fit_transform(X)
```

After fitting the PCA transformer to the dataset, its `components_` attribute holds the transpose of $\mathbf{W}_d$: it contains one row for each of the first d principal components.

Explained Variance Ratio

Another useful piece of information is the *explained variance ratio* of each principal component, available via the `explained_variance_ratio_` variable. The ratio indicates the proportion of the dataset's variance that lies along each principal component. For example, let's look at the explained variance ratios of the first two components of the 3D dataset represented in Figure 8-2:

```
>>> pca.explained_variance_ratio_
array([0.7578477 , 0.15186921])
```

This output tells you that about 76% of the dataset's variance lies along the first PC, and about 15% lies along the second PC. This leaves about 9% for the third PC, so it is reasonable to assume that the third PC probably carries little information.

Choosing the Right Number of Dimensions

Instead of arbitrarily choosing the number of dimensions to reduce down to, it is simpler to choose the number of dimensions that add up to a sufficiently large portion of the variance (e.g., 95%). Unless, of course, you are reducing dimensionality for data visualization, in which case you will want to reduce the dimensionality down to 2 or 3.

The following code loads and splits the MNIST dataset (introduced in Chapter 3) and performs PCA without reducing dimensionality, then it computes the minimum number of dimensions required to preserve 95% of the training set's variance:

```
from sklearn.datasets import fetch_openml

mnist = fetch_openml('mnist_784', as_frame=False)
```

```
X_train, y_train = mnist.data[:60_000], mnist.target[:60_000]
X_test, y_test = mnist.data[60_000:], mnist.target[60_000:]

pca = PCA()
pca.fit(X_train)
cumsum = np.cumsum(pca.explained_variance_ratio_)
d = np.argmax(cumsum >= 0.95) + 1  # d equals 154
```

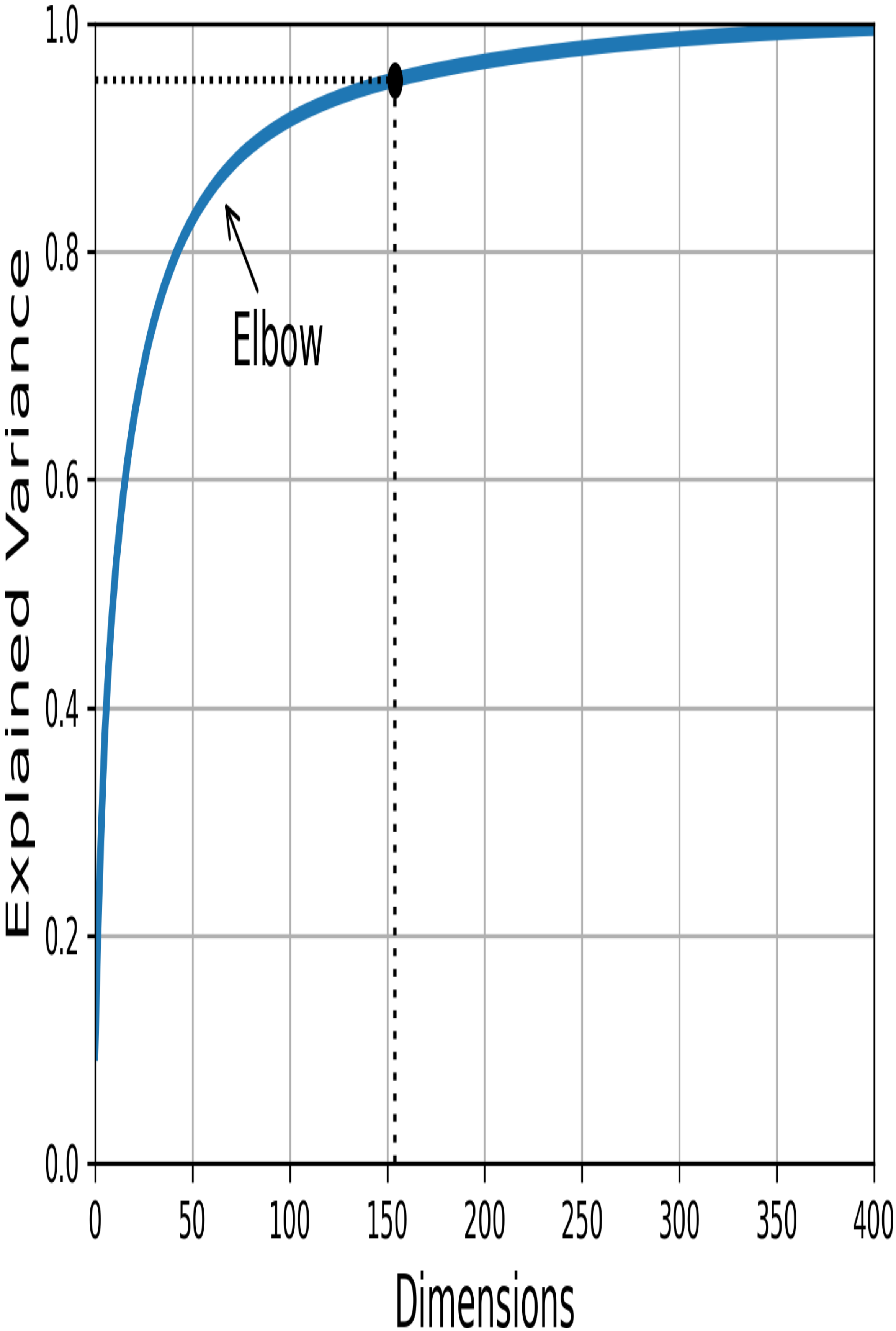
You could then set `n_components=d` and run PCA again. But there is a better option: instead of specifying the number of principal components you want to preserve, you can set `n_components` to be a float between 0.0 and 1.0, indicating the ratio of variance you wish to preserve:

```
pca = PCA(n_components=0.95)
X_reduced = pca.fit_transform(X_train)
```

The actual number of components is determined during training, and it is stored in the `n_components_` attribute:

```
>>> pca.n_components_
154
```

Yet another option is to plot the explained variance as a function of the number of dimensions (simply plot `cumsum`; see Figure 8-8). There will usually be an elbow in the curve, where the explained variance stops growing fast. In this case, you can see that reducing the dimensionality down to about 100 dimensions wouldn't lose too much explained variance.



Explained Variance
Dimensions
Elbow
1.0
0.8
0.6
0.4
0.2
0.0
0
50
100
150
200
250
300
350
400

Figure 8-8. Explained variance as a function of the number of dimensions

Lastly, if you are using dimensionality reduction as a preprocessing step for a supervised learning task (e.g., classification), then you can tune the number of dimensions as you would any other hyperparameter (see Chapter 2). For example, the following code example creates a two-step pipeline, first reducing dimensionality using PCA, then classifying using a Random Forest. Next, it uses `RandomizedSearchCV` to find a good combination of hyperparameters for both PCA and the Random Forest classifier. This example does a quick search, tuning only two hyperparameters, training on just 1,000 instances, and running for just 10 iterations, but feel free do a more thorough search if you have the time.

```
from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import RandomizedSearchCV
from sklearn.pipeline import make_pipeline

clf = make_pipeline(PCA(random_state=42),
                    RandomForestClassifier(random_state=42))
param_distrib = {
    "pca__n_components": np.arange(10, 80),
    "randomforestclassifier__n_estimators": np.arange(50, 500)
}
rnd_search = RandomizedSearchCV(clf, param_distrib, n_iter=10,
cv=3,
                                random_state=42)
rnd_search.fit(X_train[:1000], y_train[:1000])
```

Let’s look at the best hyperparameters found:

```
>>> print(rnd_search.best_params_)
{'randomforestclassifier__n_estimators': 465,
'pca__n_components': 23}
```

It’s interesting to note how low the optimal number of components is: we reduced a 784-dimensional dataset to just 23 dimensions! This is tied to the fact that we used a Random Forest, which is a pretty powerful model. If we used a linear model instead, such as an `SGDClassifier`, the search would find that we need to preserve more dimensions (about 70).

PCA for Compression

After dimensionality reduction, the training set takes up much less space. For example, after applying PCA to the MNIST dataset while preserving 95% of its variance, we are left with 154 features, instead of the original 784 features. So the dataset is now less than 20% of its original size, and we only lost 5% of its variance! This is a reasonable compression ratio, and it's easy to see how such a size reduction would speed up a classification algorithm tremendously.

It is also possible to decompress the reduced dataset back to 784 dimensions by applying the inverse transformation of the PCA projection. This won't give you back the original data, since the projection lost a bit of information (within the 5% variance that was dropped), but it will likely be close to the original data. The mean squared distance between the original data and the reconstructed data (compressed and then decompressed) is called the *reconstruction error*.

The `inverse_transform()` method lets us decompress the reduced MNIST dataset back to 784 dimensions:

```
X_recovered = pca.inverse_transform(X_reduced)
```

Figure 8-9 shows a few digits from the original training set (on the left), and the corresponding digits after compression and decompression. You can see that there is a slight image quality loss, but the digits are still mostly intact.

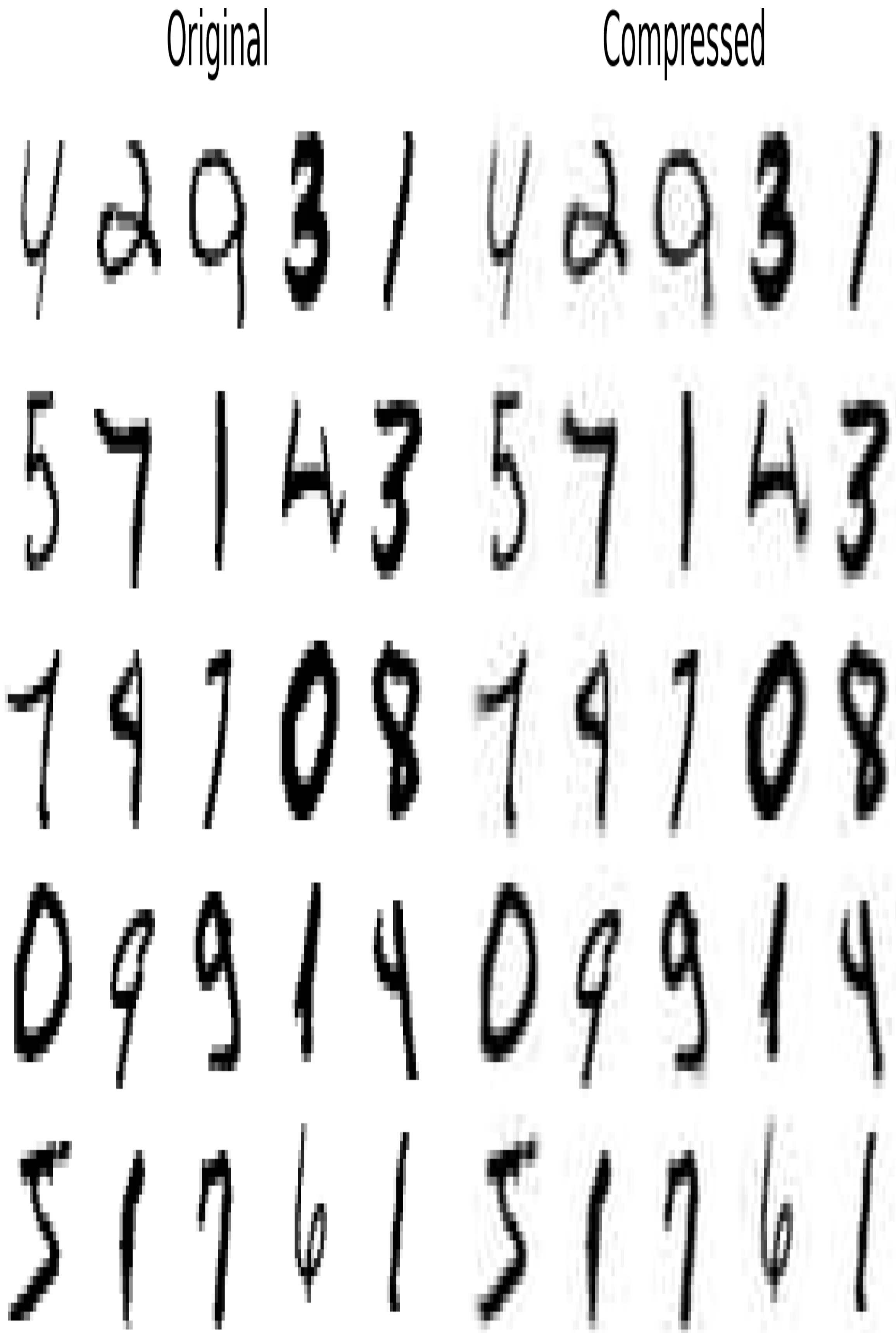

Original
Compressed

Figure 8-9. MNIST compression that preserves 95% of the variance

The equation of the inverse transformation is shown in Equation 8-3.

Equation 8-3. PCA inverse transformation, back to the original number of dimensions

$$\mathbf{X}_{\text{recovered}} = \mathbf{X}_{d\text{-proj}} \mathbf{W}_d^{\intercal}$$

Randomized PCA

If you set the `svd_solver` hyperparameter to `"randomized"`, Scikit-Learn uses a stochastic algorithm called *Randomized PCA* that quickly finds an approximation of the first *d* principal components. Its computational complexity is $O(m \times d^2) + O(d^3)$, instead of $O(m \times n^2) + O(n^3)$ for the full SVD approach, so it is dramatically faster than full SVD when *d* is much smaller than *n*:

```
rnd_pca = PCA(n_components=154, svd_solver="randomized",
random_state=42)
X_reduced = rnd_pca.fit_transform(X_train)
```

> **TIP**
>
> By default, `svd_solver` is actually set to `"auto"`: Scikit-Learn automatically uses the randomized PCA algorithm if max(m, n) > 500 and `n_components` is an integer smaller than 80% of min(m, n), or else it uses the full SVD approach. So the preceding code would use the randomized PCA algorithm even if you removed `svd_solver="randomized"` argument, since 154 < 0.8 × 784. If you want to force Scikit-Learn to use full SVD, you can set the `svd_solver` hyperparameter to `"full"`.

Incremental PCA

One problem with the preceding implementations of PCA is that they require the whole training set to fit in memory in order for the algorithm to run. Fortunately, *Incremental PCA* (IPCA) algorithms have been developed. They allow you to split the training set into mini-batches and feed an IPCA algorithm one mini-batch at a time. This is useful for large training sets and for applying PCA online (i.e., on the fly, as new instances arrive).

The following code splits the MNIST training set into 100 mini-batches (using NumPy's `array_split()` function) and feeds them to Scikit-Learn's `IncrementalPCA` class[5] to reduce the dimensionality of the MNIST dataset down to 154 dimensions, just like before. Note that you must call the `partial_fit()` method with each mini-batch, rather than the `fit()` method with the whole training set:

```
from sklearn.decomposition import IncrementalPCA

n_batches = 100
inc_pca = IncrementalPCA(n_components=154)
for X_batch in np.array_split(X_train, n_batches):
    inc_pca.partial_fit(X_batch)

X_reduced = inc_pca.transform(X_train)
```

Alternatively, you can use NumPy's `memmap` class, which allows you to manipulate a large array stored in a binary file on disk as if it were entirely in memory; the class loads only the data it needs in memory, when it needs it. To demonstrate this, let's first create a memmap file and copy the MNIST training set to it, then call `flush()` to ensure that any data still in cache gets saved to disk. In real life, `X_train` would typically not fit in memory so you would load it chunk by chunk and save each chunk to the right part of the memmap array:

```
filename = "my_mnist.mmap"
X_mmap = np.memmap(filename, dtype='float32', mode='write',
shape=X_train.shape)
X_mmap[:] = X_train  # could be a loop instead, saving the data
chunk by chunk
X_mmap.flush()
```

Next, we can load the memmap file and use it like a regular NumPy array. Let's use the `IncrementalPCA` class to reduce its dimensionality. Since this algorithm uses only a small part of the array at any given time, memory usage remains under control. This makes it possible to call the usual `fit()` method instead of `partial_fit()`, which is quite convenient:

```
X_mmap = np.memmap(filename, dtype="float32",
mode="readonly").reshape(-1, 784)
batch_size = X_mmap.shape[0] // n_batches
inc_pca = IncrementalPCA(n_components=154, batch_size=batch_size)
inc_pca.fit(X_mmap)
```

> **WARNING**
>
> Only the raw binary data is saved to disk, so you need to specify the data type and shape of the array when you load it. If you omit the shape, `np.memmap()` returns a 1D array.

For very high-dimensional datasets, PCA can be too slow. As we saw earlier, even if you use Randomized PCA, its computational complexity is still $O(m \times d^2) + O(d^3)$, so the target number of dimensions d must not be too large. If you are dealing with a dataset with tens of thousands of features or more (e.g., images), then training may become much too slow: in this case, you should consider using Random Projection instead.

Random Projection

As its name suggests, the Random Projection algorithm projects the data to a lower-dimensional space using a random linear projection. This may sound crazy, but it turns out that such a random projection is actually very likely to preserve distances fairly well, as was demonstrated mathematically by William B. Johnson and Joram Lindenstrauss in a famous lemma. So two similar instances will remain similar after the projection, and two very different instances will remain very different.

Obviously, the more dimensions you drop, the more information is lost, and the more distances get distorted. So how can you choose the optimal number of dimensions? Well, Johnson and Lindenstrauss came up with an equation that determines the minimum number of dimensions to preserve in order to ensure—with high probability—that distances won't change by more than a given tolerance. For example, if you have a dataset containing m = 5,000 instances with n = 20,000 features each, and you don't want the squared distance between any two instances to change by more than ε = 10%,[6] then you should project the data down to d dimensions, with $d \geq 4 \log(m) / (\frac{1}{2} \varepsilon^2 - \frac{1}{3} \varepsilon^3)$, which is 7,300 dimensions. That's quite a significant dimensionality reduction! Notice that the equation does not use n, it only relies on m and ε. This equation is implemented by the `johnson_lindenstrauss_min_dim()` function:

```
>>> from sklearn.random_projection import
johnson_lindenstrauss_min_dim
>>> m, ε = 5_000, 0.1
>>> d = johnson_lindenstrauss_min_dim(m, eps=ε)
>>> d
7300
```

Now we can just generate a random matrix **P** of shape [d, n], where each item is sampled randomly from a Gaussian distribution with mean 0 and variance 1 / d, and we use it to project a dataset from n dimensions down to d:

```
n = 20_000
np.random.seed(42)
P = np.random.randn(d, n) / np.sqrt(d)  # std dev = square root
of variance

X = np.random.randn(m, n)  # generate a fake dataset
X_reduced = X @ P.T
```

That's all there is to it! It's simple and efficient, and no training is required: the only thing the algorithm needs to create the random matrix is the dataset's shape, that's it. The data itself is not used at all.

Scikit-Learn offers a `GaussianRandomProjection` class to do exactly what we just did: when you call its `fit()` method, it uses `johnson_lindenstrauss_min_dim()` to determine the output dimensionality, then it generates a random matrix, which it stores in the `components_` attribute. Then when you call `transform()`, it uses this matrix to perform the projection. When creating the transformer, you can set `eps` if you want to tweak ε (it defaults to 0.1), and `n_components` if you want to force a specific target dimensionality d. The following code example gives the same result as above (you can also verify that `gaussian_rnd_proj.components_` is equal to `P`):

```
from sklearn.random_projection import GaussianRandomProjection

gaussian_rnd_proj = GaussianRandomProjection(eps=ε,
random_state=42)
X_reduced = gaussian_rnd_proj.fit_transform(X)  # same result as
above
```

Scikit-Learn provides a second random projection transformer: `SparseRandomProjection`. It determines the target dimensionality in the same way, it generates a random matrix of the same shape, and it performs the projection identically. The main difference is that the random matrix is sparse. This means it uses much less memory: about 25 MB instead of almost 1.2GB in the preceding example! And it's also much faster, both to generate the random matrix and to reduce dimensionality: about 50% faster on the preceding example. Moreover, if the input is sparse, the transformation keeps it sparse (unless you set `dense_output=True`). Lastly, it enjoys the same distance-preserving property as the previous approach, and the quality of the dimensionality reduction is comparable. In short, it's usually preferable to use this transformer instead of the first one, especially for large or sparse datasets.

The ratio r of nonzero items in the sparse random matrix is called its *density*. By default, it is equal to $1/\sqrt{n}$. With 20,000 features, this means that only one in ~141 cells in the random matrix is nonzero: that's quite sparse! You can set the `density` hyperparameter to another value if you prefer. Each cell in the sparse random matrix has a probability r of being nonzero, and each nonzero value is either $-v$ or $+v$ (both equally likely), where $v = 1/\sqrt{dr}$.

NOTE

Random Projection is not always used to reduce the dimensionality of large datasets. For example, a 2017 paper[7] by Sanjoy Dasgupta et al. showed that the brain of fruit flies implements an analog of Random Projection to map dense low-dimensional olfactory inputs to sparse high-dimensional binary outputs: for each odor, only a small fraction of the output neurons get activated, but similar odors activate many of the same neurons. This is similar to a well-known algorithm called *Locality Sensitive Hashing* (LSH) which is typically used in search engines to group similar documents.

If you want to perform the inverse transform, you first need to compute the pseudo-inverse of the components matrix, using SciPy's `pinv()` function, then multiply the reduced data by the transpose of the pseudo-inverse:

```
components_pinv = np.linalg.pinv(gaussian_rnd_proj.components_)
X_recovered = X_reduced @ components_pinv.T
```

WARNING

Computing the pseudo-inverse may take a very long time if the components matrix is large, as the computational complexity of `pinv()` is $\mathcal{O}(dn^2)$ if $d < n$, or $\mathcal{O}(nd^2)$ otherwise.

In summary, Random Projection is a simple, fast, memory-efficient and surprisingly powerful dimensionality reduction algorithm that you should keep in mind, especially when you deal with high-dimensional datasets.

LLE

Locally Linear Embedding (LLE)[8] is a *nonlinear dimensionality reduction* (NLDR) technique. It is a Manifold Learning technique that does not rely on projections, unlike PCA and Random Projection. In a nutshell, LLE works by first measuring how each training instance linearly relates to its nearest neighbors, and then looking for a low-dimensional representation of the training set where these local relationships are best preserved (more details shortly). This approach makes it particularly good at unrolling twisted manifolds, especially when there is not too much noise.

The following code makes a Swiss roll then uses Scikit-Learn's `LocallyLinearEmbedding` class to unroll it:

```
from sklearn.datasets import make_swiss_roll
from sklearn.manifold import LocallyLinearEmbedding

X_swiss, t = make_swiss_roll(n_samples=1000, noise=0.2,
random_state=42)
lle = LocallyLinearEmbedding(n_components=2, n_neighbors=10,
random_state=42)
X_unrolled = lle.fit_transform(X_swiss)
```

The variable `t` is a 1D NumPy array containing the position of each instance along the rolled axis of Swiss roll. We don't use it in this example, but it can be used as a target for a non-linear regression task.

The resulting 2D dataset is shown in Figure 8-10. As you can see, the Swiss roll is completely unrolled, and the distances between instances are locally well preserved. However, distances are not preserved on a larger scale: the unrolled Swiss roll should be a rectangle, not this kind of stretched and twisted band. Nevertheless, LLE did a pretty good job at modeling the manifold.

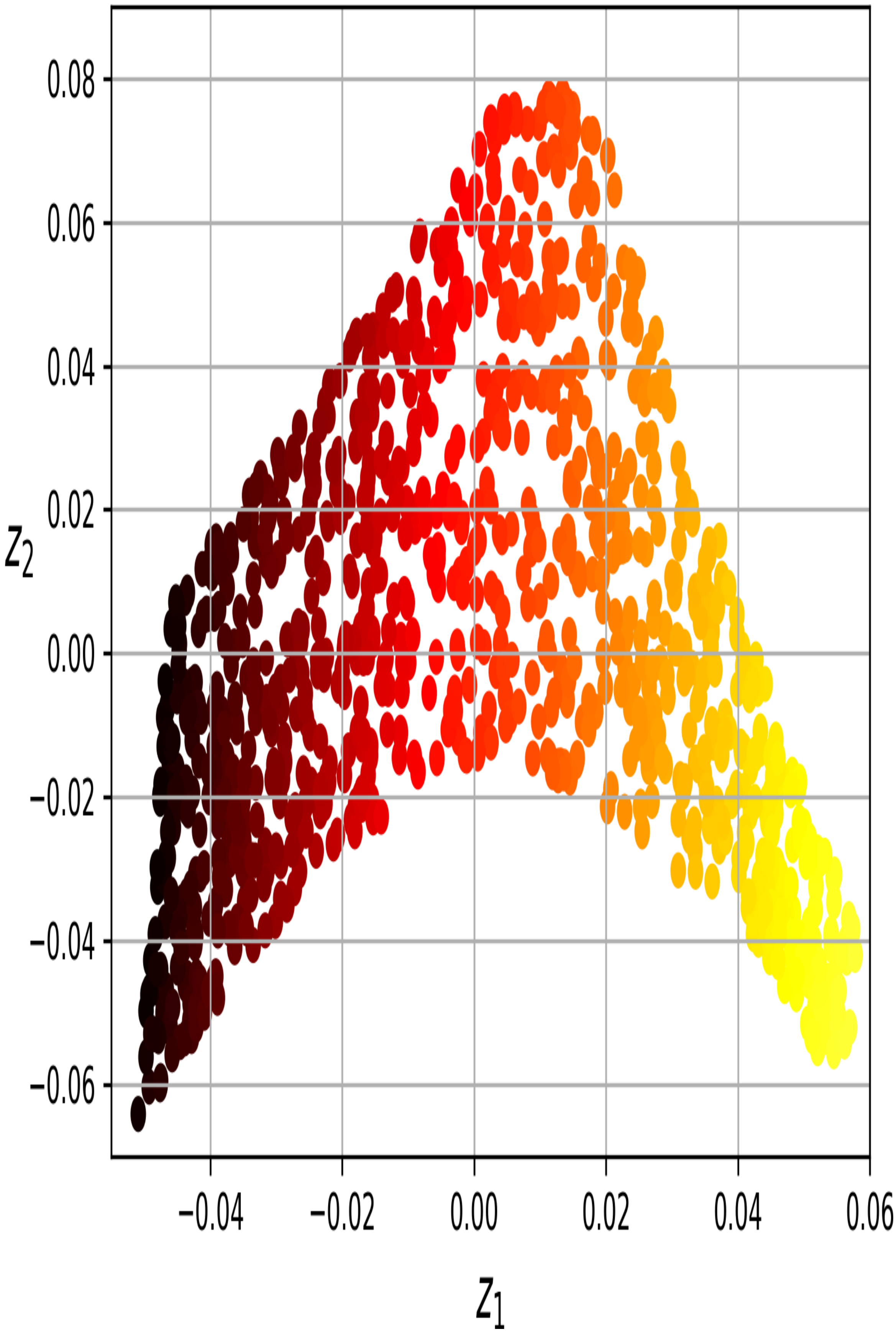

0.08
0.06
0.04
0.02
0.00
−0.02
−0.04
−0.06
z_2
−0.04
−0.02
0.00
0.02
0.04
0.06
z_1

Figure 8-10. Unrolled Swiss roll using LLE

Here's how LLE works: for each training instance $\mathbf{x}^{(i)}$, the algorithm identifies its k nearest neighbors (in the preceding code $k = 10$), then tries to reconstruct $\mathbf{x}^{(i)}$ as a linear function of these neighbors. More specifically, it tries to find the weights $w_{i,j}$ such that the squared distance between $\mathbf{x}^{(i)}$ and $\sum_{j=1}^{m} w_{i,j}\mathbf{x}^{(j)}$ is as small as possible, assuming $w_{i,j} = 0$ if $\mathbf{x}^{(j)}$ is not one of the k nearest neighbors of $\mathbf{x}^{(i)}$. Thus the first step of LLE is the constrained optimization problem described in Equation 8-4, where $\mathbf{W}$ is the weight matrix containing all the weights $w_{i,j}$. The second constraint simply normalizes the weights for each training instance $\mathbf{x}^{(i)}$.

Equation 8-4. LLE step one: linearly modeling local relationships

$$\widehat{\mathbf{W}} = \underset{\mathbf{W}}{\operatorname{argmin}} \sum_{i=1}^{m} \left(\mathbf{x}^{(i)} - \sum_{j=1}^{m} w_{i,j}\mathbf{x}^{(j)} \right)^2$$

$$\text{subject to } \begin{cases} w_{i,j} = 0 & \text{if } \mathbf{x}^{(j)} \text{ is not one of the } k \text{ n.n. of } \mathbf{x}^{(i)} \\ \sum_{j=1}^{m} w_{i,j} = 1 & \text{for } i = 1, 2, \cdots, m \end{cases}$$

After this step, the weight matrix $\widehat{\mathbf{W}}$ (containing the weights $\widehat{w}_{i,j}$) encodes the local linear relationships between the training instances. The second step is to map the training instances into a d-dimensional space (where $d < n$) while preserving these local relationships as much as possible. If $\mathbf{z}^{(i)}$ is the image of $\mathbf{x}^{(i)}$ in this d-dimensional space, then we want the squared distance between $\mathbf{z}^{(i)}$ and $\sum_{j=1}^{m} \widehat{w}_{i,j}\mathbf{z}^{(j)}$ to be as small as possible. This idea leads to the unconstrained optimization problem described in Equation 8-5. It looks very similar to the first step, but instead of keeping the instances fixed and finding the optimal weights, we are doing the reverse: keeping the weights fixed and finding the optimal position of the instances' images in the low-dimensional space. Note that $\mathbf{Z}$ is the matrix containing all $\mathbf{z}^{(i)}$.

Equation 8-5. LLE step two: reducing dimensionality while preserving relationships

$$\widehat{\mathbf{Z}} = \underset{\mathbf{Z}}{\operatorname{argmin}} \sum_{i=1}^{m} \left(\mathbf{z}^{(i)} - \sum_{j=1}^{m} \widehat{w}_{i,j} \mathbf{z}^{(j)} \right)^2$$

Scikit-Learn's LLE implementation has the following computational complexity: $\mathcal{O}(m \log(m) n \log(k))$ for finding the k nearest neighbors, $\mathcal{O}(mnk^3)$ for optimizing the weights, and $\mathcal{O}(dm^2)$ for constructing the low-dimensional representations. Unfortunately, the m^2 in the last term makes this algorithm scale poorly to very large datasets.

As you can see, LLE is quite different from the projection techniques, and it's significantly more complex, but it can also perform much better, especially if the data is non-linear.

Before we conclude this chapter, let's take a quick look at a few other popular dimensionality reduction techniques available in Scikit-Learn:

`sklearn.manifold.MDS` *Multidimensional Scaling* (MDS) reduces dimensionality while trying to preserve the distances between the instances. Random Projection does that for high-dimensional data, but it doesn't work well on low-dimensional data. `sklearn.manifold.Isomap` *Isomap* creates a graph by connecting each instance to its nearest neighbors, then reduces dimensionality while trying to preserve the *geodesic distances* between the instances. The geodesic distance between two nodes in a graph is the number of nodes on the shortest path between these nodes. `sklearn.manifold.TSNE` *t-Distributed Stochastic Neighbor Embedding* (t-SNE) reduces dimensionality while trying to keep similar instances close and dissimilar instances apart. It is mostly used for visualization, in particular to visualize clusters of instances in high-dimensional space. For example, in the exercises at the end of this chapter you will use t-SNE to visualize a 2D map of the MNIST images. `sklearn.discriminant_analysis.LinearDiscriminantAnalysis` *Linear Discriminant Analysis* (LDA) is a linear classification algorithm, and during training it learns the most discriminative axes between the classes. These axes can then be used to define a hyperplane onto which to project the data. The benefit of this approach is that the projection will keep classes as far apart as possible, so LDA is a good technique to reduce dimensionality before running another classification algorithm (unless LDA is sufficient).

Figure 8-11 shows the results of MDS, Isomap and t-SNE on the Swiss roll.

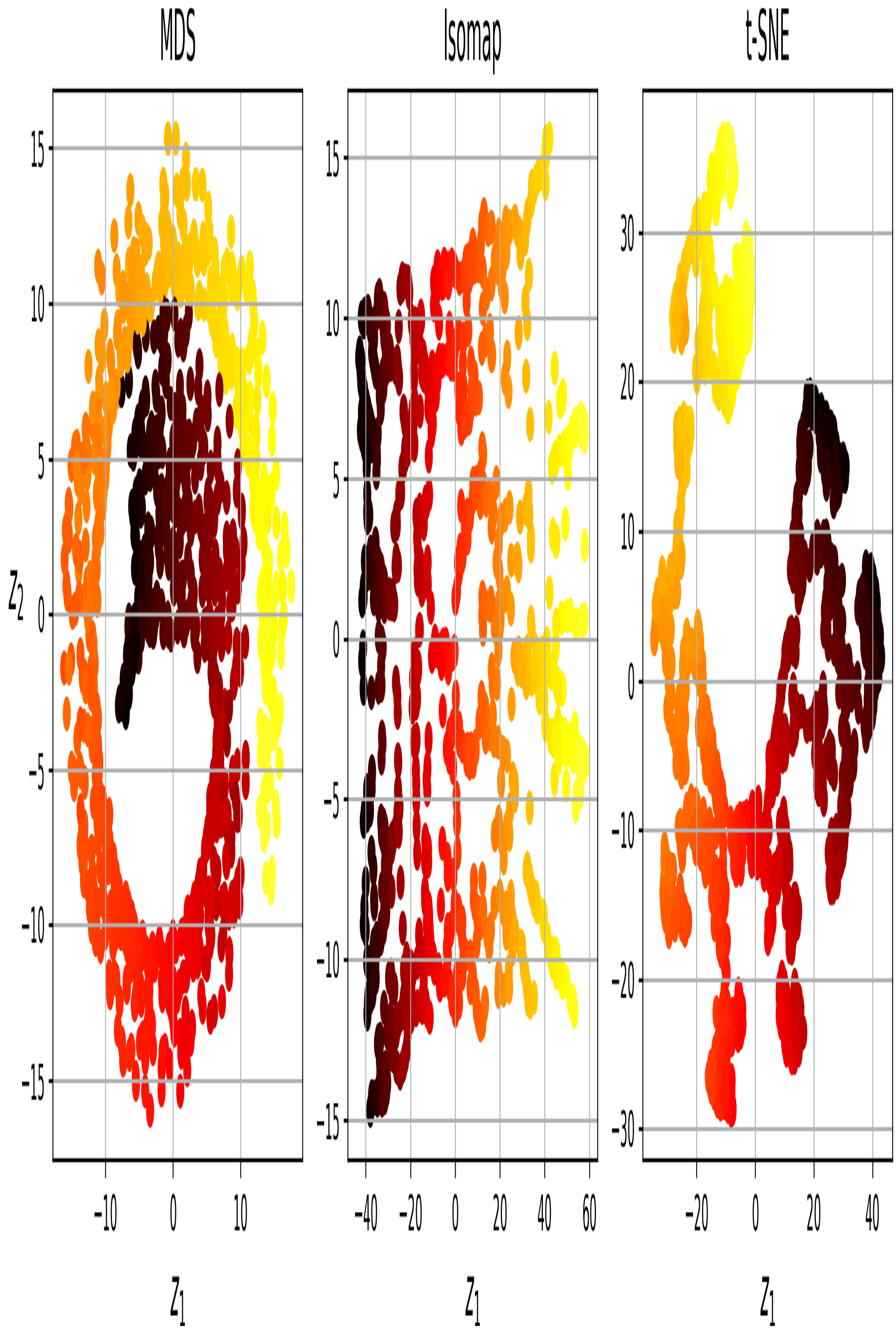

MDS
Isomap
t-SNE
z_2
z_1
z_1
z_1
15
10
5
0
-5
-10
-15
-10
0
10
-40
-20
0
20
40
60
30
20
10
0
-10
-20
-30
-20
0
20
40

Figure 8-11. Using various techniques to reduce the Swiss roll to 2D

Exercises

1. What are the main motivations for reducing a dataset's dimensionality? What are the main drawbacks?

2. What is the curse of dimensionality?

3. Once a dataset's dimensionality has been reduced, is it possible to reverse the operation? If so, how? If not, why?

4. Can PCA be used to reduce the dimensionality of a highly nonlinear dataset?

5. Suppose you perform PCA on a 1,000-dimensional dataset, setting the explained variance ratio to 95%. How many dimensions will the resulting dataset have?

6. In what cases would you use regular PCA, Incremental PCA, Randomized PCA, or Random Projection?

7. How can you evaluate the performance of a dimensionality reduction algorithm on your dataset?

8. Does it make any sense to chain two different dimensionality reduction algorithms?

9. Load the MNIST dataset (introduced in Chapter 3) and split it into a training set and a test set (take the first 60,000 instances for training, and the remaining 10,000 for testing). Train a Random Forest classifier on the dataset and time how long it takes, then evaluate the resulting model on the test set. Next, use PCA to reduce the dataset's dimensionality, with an explained variance ratio of 95%. Train a new Random Forest classifier on the reduced dataset and see how long it takes. Was training much faster? Next, evaluate the classifier on the test set. How does it compare to the

previous classifier? Try again with an `SGDClassifier`. How much does PCA help now?

10. Use t-SNE to reduce the first 5,000 images of the MNIST dataset down to two dimensions and plot the result using Matplotlib. You can use a scatterplot using 10 different colors to represent each image's target class. Alternatively, you can replace each dot in the scatterplot with the corresponding instance's class (a digit from 0 to 9), or even plot scaled-down versions of the digit images themselves (if you plot all digits, the visualization will be too cluttered, so you should either draw a random sample or plot an instance only if no other instance has already been plotted at a close distance). You should get a nice visualization with well-separated clusters of digits. Try using other dimensionality reduction algorithms such as PCA, LLE, or MDS and compare the resulting visualizations.

Solutions to these exercises are available at the end of this chapter's notebook, at *https://homl.info/colab3*.

---

1 Well, four dimensions if you count time, and a few more if you are a string theorist.

2 Watch a rotating tesseract projected into 3D space at *https://homl.info/30*. Image by Wikipedia user NerdBoy1392 (Creative Commons BY-SA 3.0). Reproduced from *https://en.wikipedia.org/wiki/Tesseract*.

3 Fun fact: anyone you know is probably an extremist in at least one dimension (e.g., how much sugar they put in their coffee), if you consider enough dimensions.

4 Karl Pearson, "On Lines and Planes of Closest Fit to Systems of Points in Space," *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science* 2, no. 11 (1901): 559-572, *https://homl.info/pca*.

5 Scikit-Learn uses the algorithm described in David A. Ross et al., "Incremental Learning for Robust Visual Tracking," *International Journal of Computer Vision* 77, no. 1–3 (2008): 125–141.

6 ε is the greek letter epsilon, often used for tiny values.

7 Sanjoy Dasgupta et al., "A neural algorithm for a fundamental computing problem," *Science* 358, no. 6364 (2017): 793–796.

8 Sam T. Roweis and Lawrence K. Saul, “Nonlinear Dimensionality Reduction by Locally Linear Embedding,” *Science* 290, no. 5500 (2000): 2323–2326.

Chapter 9. Unsupervised Learning Techniques

> **A NOTE FOR EARLY RELEASE READERS**
>
> With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.
>
> This will be the 9th chapter of the final book. Notebooks are available on GitHub at *https://github.com/ageron/handson-ml3*. Datasets are available at *https://github.com/ageron/data*.
>
> If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the editoor at ntache@oreilly.com.

Although most of the applications of Machine Learning today are based on supervised learning (and as a result, this is where most of the investments go to), the vast majority of the available data is unlabeled: we have the input features **X**, but we do not have the labels **y**. The computer scientist Yann LeCun famously said that "if intelligence was a cake, unsupervised learning would be the cake, supervised learning would be the icing on the cake, and reinforcement learning would be the cherry on the cake." In other words, there is a huge potential in unsupervised learning that we have only barely started to sink our teeth into.

Say you want to create a system that will take a few pictures of each item on a manufacturing production line and detect which items are defective. You can fairly easily create a system that will take pictures automatically, and this might give you thousands of pictures every day. You can then build a reasonably large dataset in just a few weeks. But wait, there are no labels! If you want to train a regular binary classifier that will predict whether an item is defective or not, you will need to label every single picture as "defective" or "normal." This will generally require human experts to sit down and manually go through all the pictures. This is a long, costly, and tedious task, so it will usually only be done on a small subset of the available pictures. As a result, the labeled dataset will be quite small, and the classifier's performance will be disappointing. Moreover, every time the company makes any change to its products, the whole process will need to be started over from scratch. Wouldn't it be great if the algorithm could just exploit the unlabeled data without needing humans to label every picture? Enter unsupervised learning.

In Chapter 8 we looked at the most common unsupervised learning task: dimensionality reduction. In this chapter we will look at a few more unsupervised learning tasks and algorithms:

Clustering

The goal is to group similar instances together into *clusters*. Clustering is a great tool for data analysis, customer segmentation, recommender systems, search engines, image segmentation, semi-supervised learning, dimensionality reduction, and more.

Anomaly detection

The objective is to learn what "normal" data looks like, and then use that to detect abnormal instances, such as defective items on a production line or a new trend in a time series.

Density estimation

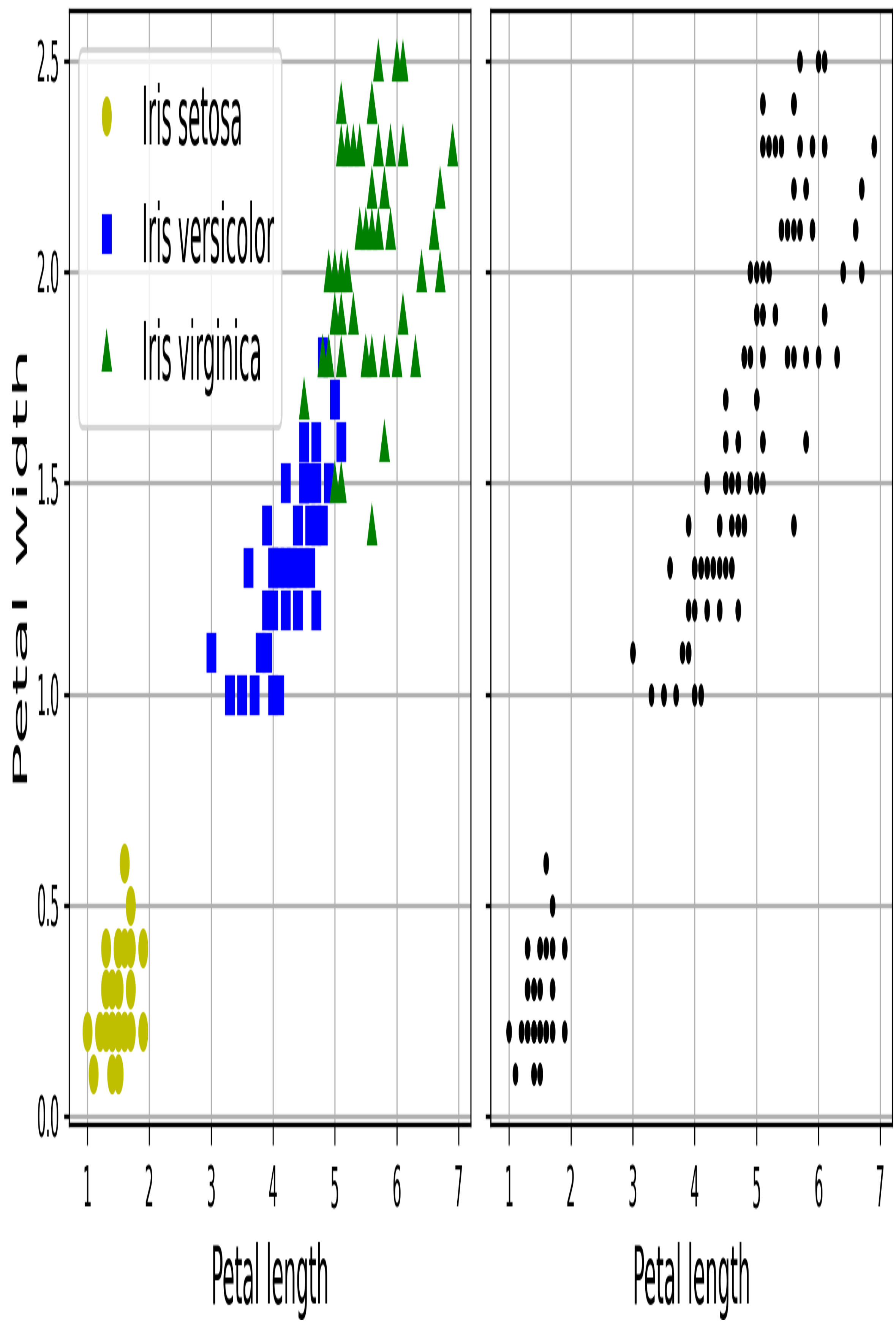
This is the task of estimating the *probability density function* (PDF) of the random process that generated the dataset. Density estimation is commonly used for anomaly detection: instances located in very low-density regions are likely to be anomalies. It is also useful for data analysis and visualization.

Ready for some cake? We will start with clustering, using K-Means and DBSCAN, and then we will discuss Gaussian mixture models and see how they can be used for density estimation, clustering, and anomaly detection.

Clustering

As you enjoy a hike in the mountains, you stumble upon a plant you have never seen before. You look around and you notice a few more. They are not identical, yet they are sufficiently similar for you to know that they most likely belong to the same species (or at least the same genus). You may need a botanist to tell you what species that is, but you certainly don't need an expert to identify groups of similar-looking objects. This is called *clustering*: it is the task of identifying similar instances and assigning them to *clusters*, or groups of similar instances.

Just like in classification, each instance gets assigned to a group. However, unlike classification, clustering is an unsupervised task. Consider Figure 9-1: on the left is the iris dataset (introduced in Chapter 4), where each instance's species (i.e., its class) is represented with a different marker. It is a labeled dataset, for which classification algorithms such as Logistic Regression, SVMs, or Random Forest classifiers are well suited. On the right is the same dataset, but without the labels, so you cannot use a classification algorithm anymore. This is where clustering algorithms step in: many of them can easily detect the lower-left cluster. It is also quite easy to see with our own eyes, but it is not so obvious that the upper-right cluster is composed of two distinct sub-clusters. That said, the dataset has two additional features (sepal length and width), not represented here, and clustering algorithms can make good use of all features, so in fact they identify the three clusters fairly well (e.g., using a Gaussian mixture model, only 5 instances out of 150 are assigned to the wrong cluster).



Iris setosa
Iris versicolor
Iris virginica
Petal width
Petal length
Petal length
0.0
0.5
1.0
1.5
2.0
2.5
1
2
3
4
5
6
7

Figure 9-1. Classification (left) versus clustering (right)

Clustering is used in a wide variety of applications, including these:

For customer segmentation

You can cluster your customers based on their purchases and their activity on your website. This is useful to understand who your customers are and what they need, so you can adapt your products and marketing campaigns to each segment. For example, customer segmentation can be useful in *recommender systems* to suggest content that other users in the same cluster enjoyed.

For data analysis

When you analyze a new dataset, it can be helpful to run a clustering algorithm, and then analyze each cluster separately.

As a dimensionality reduction technique

Once a dataset has been clustered, it is usually possible to measure each instance's *affinity* with each cluster: affinity is any measure of how well an instance fits into a cluster. Each instance's feature vector **x** can then be replaced with the vector of its cluster affinities. If there are *k* clusters, then this vector is *k*-dimensional. This vector is typically much lower-dimensional than the original feature vector, but it can preserve enough information for further processing.

For feature engineering

The cluster affinities can often be useful as extra features. For example, we used K-Means in Chapter 2 to add geographic cluster affinity features to the California housing dataset, and they helped us get better performance.

For anomaly detection (also called outlier detection)

Any instance that has a low affinity to all the clusters is likely to be an anomaly. For example, if you have clustered the users of your website based on their behavior, you can detect users with unusual behavior, such as an unusual number of requests per second. Anomaly detection is particularly useful in detecting defects in manufacturing, or for *fraud detection*.

For semi-supervised learning

If you only have a few labels, you could perform clustering and propagate the labels to all the instances in the same cluster. This technique can greatly increase the number of labels available for a subsequent supervised learning algorithm, and thus improve its performance.

For search engines

Some search engines let you search for images that are similar to a reference image. To build such a system, you would first apply a clustering algorithm to all the images in your database; similar images would end up in the same cluster. Then when a user provides a reference image, all you need to do is use the trained clustering model to find this image's cluster, and you can then simply return all the images from this cluster.

To segment an image

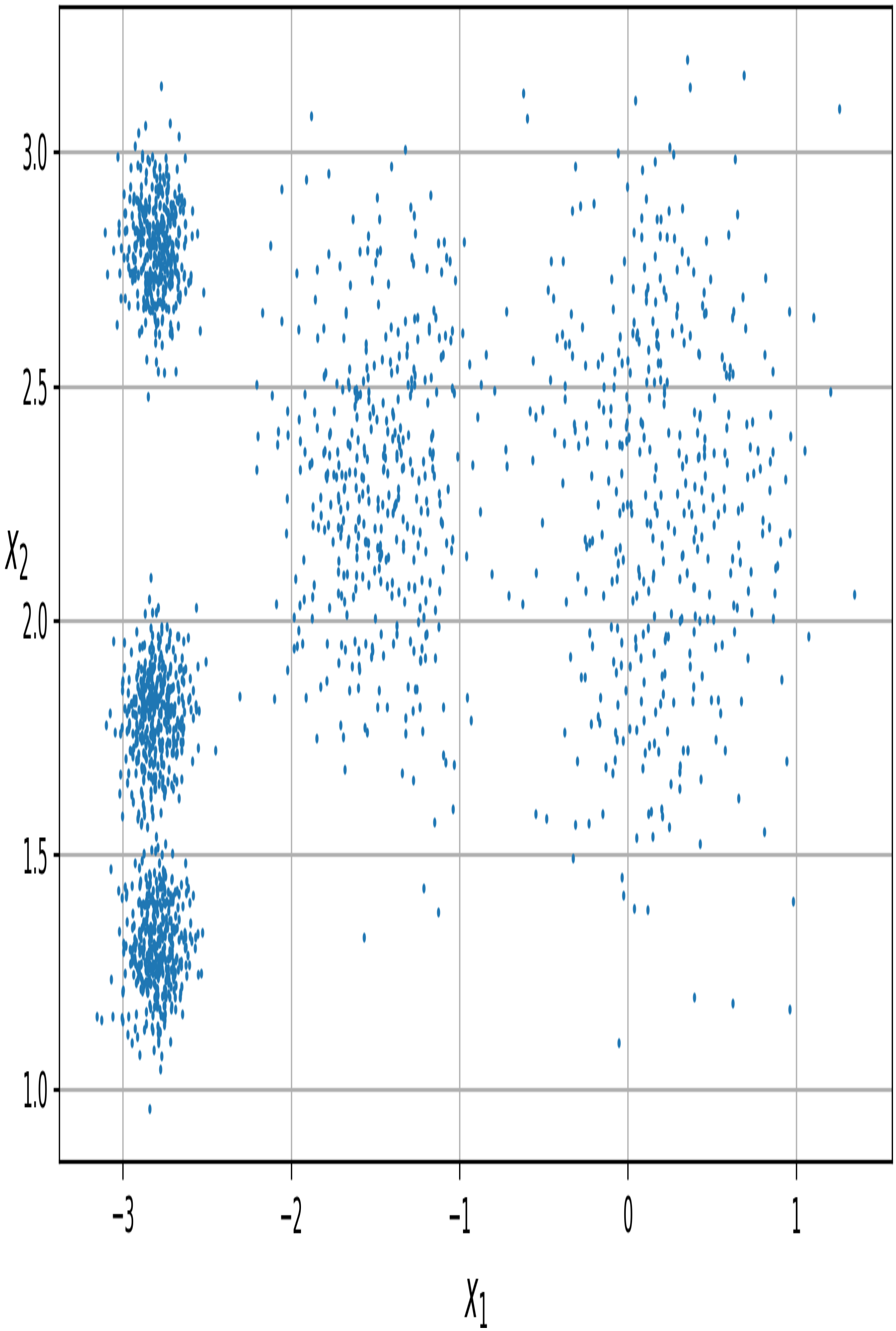
By clustering pixels according to their color, then replacing each pixel's color with the mean color of its cluster, it is possible to considerably reduce the number of different colors in the image. Image segmentation is used in many object detection and tracking systems, as it makes it easier to detect the contour of each object.

There is no universal definition of what a cluster is: it really depends on the context, and different algorithms will capture different kinds of clusters. Some algorithms look for instances centered around a particular point, called a *centroid*. Others look for continuous regions of densely packed instances: these clusters can take on any shape. Some algorithms are hierarchical, looking for clusters of clusters. And the list goes on.

In this section, we will look at two popular clustering algorithms, K-Means and DBSCAN, and explore some of their applications, such as nonlinear dimensionality reduction, semi-supervised learning, and anomaly detection.

K-Means

Consider the unlabeled dataset represented in Figure 9-2: you can clearly see five blobs of instances. The K-Means algorithm is a simple algorithm capable of clustering this kind of dataset very quickly and efficiently, often in just a few iterations. It was proposed by Stuart Lloyd at Bell Labs in 1957 as a technique for pulse-code modulation, but it was only published outside of the company in 1982.[1] In 1965, Edward W. Forgy had published virtually the same algorithm, so K-Means is sometimes referred to as Lloyd–Forgy.



3.0
2.5
2.0
1.5
1.0
X_2
-3
-2
-1
0
1
X_1

Figure 9-2. An unlabeled dataset composed of five blobs of instances

Let's train a K-Means clusterer on this dataset. It will try to find each blob's center and assign each instance to the closest blob:

```
from sklearn.cluster import KMeans
from sklearn.datasets import make_blobs

X, y = make_blobs([...])  # make the blobs: y contains the cluster ids, but we
                          # will not use them, it's what we want to predict
k = 5
kmeans = KMeans(n_clusters=k, random_state=42)
y_pred = kmeans.fit_predict(X)
```

Note that you have to specify the number of clusters *k* that the algorithm must find. In this example, it is pretty obvious from looking at the data that *k* should be set to 5, but in general it is not that easy. We will discuss this shortly.

Each instance was assigned to one of the five clusters. In the context of clustering, an instance's *label* is the index of the cluster that this instance gets assigned to by the algorithm: this is not to be confused with the class labels in classification, which are used as targets (remember that clustering is an unsupervised learning task). The `KMeans` instance preserves the predicted labels of the instances it was trained on, available via the `labels_` instance variable:

```
>>> y_pred
array([4, 0, 1, ..., 2, 1, 0], dtype=int32)
>>> y_pred is kmeans.labels_
True
```

We can also take a look at the five centroids that the algorithm found:

```
>>> kmeans.cluster_centers_
array([[-2.80389616,  1.80117999],
       [ 0.20876306,  2.25551336],
       [-2.79290307,  2.79641063],
```

```
         [-1.46679593,  2.28585348],
         [-2.80037642,  1.30082566]])
```

You can easily assign new instances to the cluster whose centroid is closest:

```
>>> import numpy as np
>>> X_new = np.array([[0, 2], [3, 2], [-3, 3], [-3, 2.5]])
>>> kmeans.predict(X_new)
array([1, 1, 2, 2], dtype=int32)
```

If you plot the cluster's decision boundaries, you get a Voronoi tessellation: see Figure 9-3, where each centroid is represented with an X.

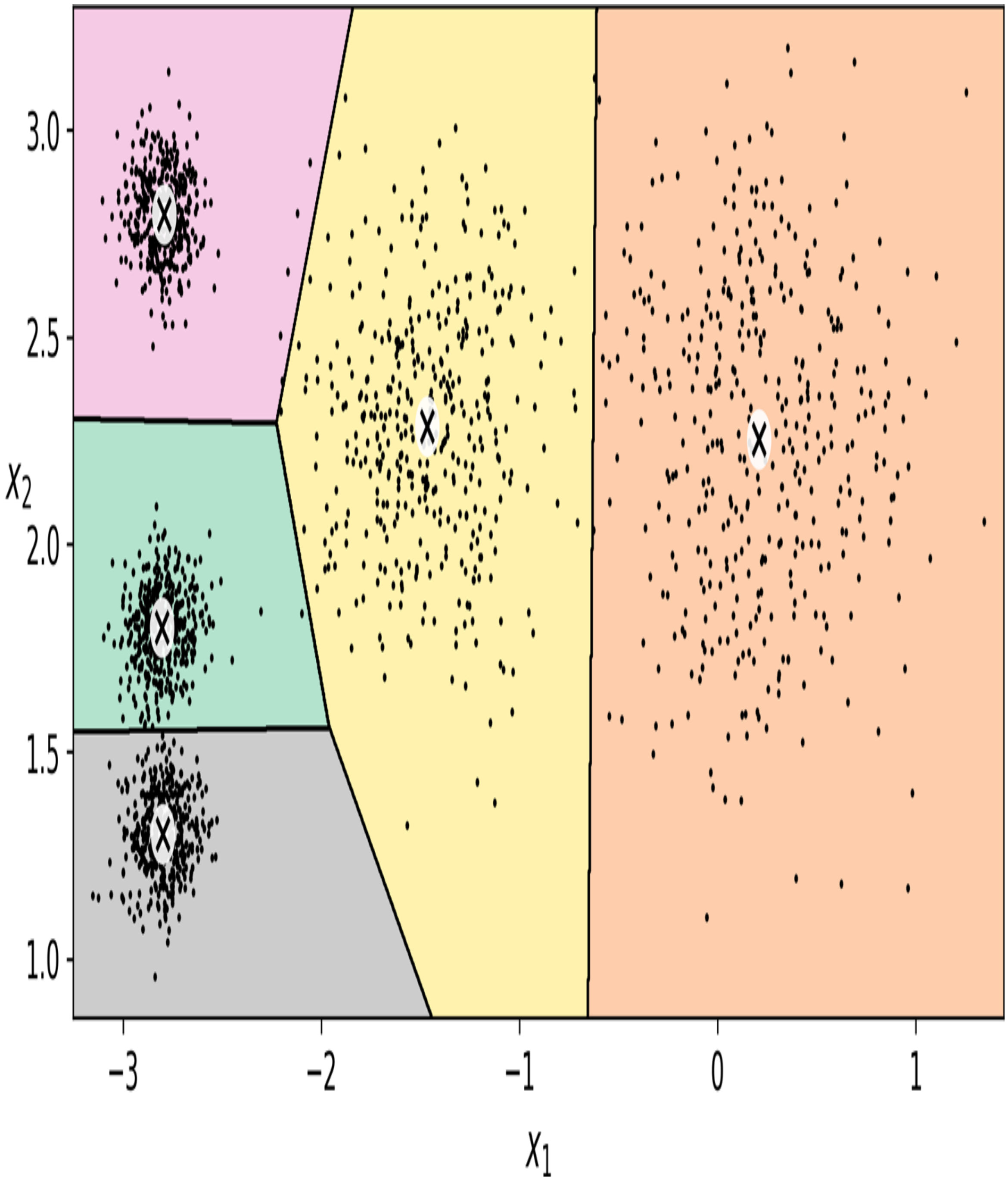


Figure 9-3. K-Means decision boundaries (Voronoi tessellation)

The vast majority of the instances were clearly assigned to the appropriate cluster, but a few instances were probably mislabeled, especially near the boundary between the top-left cluster and the central cluster. Indeed, the K-Means algorithm does not behave very well when the blobs have very different diameters because all it cares about when assigning an instance to a cluster is the distance to the centroid.

Instead of assigning each instance to a single cluster, which is called *hard clustering*, it can be useful to give each instance a score per cluster, which is called *soft clustering*. The score can be the distance between the instance and the centroid; conversely, it can be a similarity score (or affinity), such as the Gaussian Radial Basis Function we used in Chapter 2. In the `KMeans` class, the `transform()` method measures the distance from each instance to every centroid:

```
>>> kmeans.transform(X_new).round(2)
array([[2.81, 0.33, 2.9 , 1.49, 2.89],
       [5.81, 2.8 , 5.85, 4.48, 5.84],
       [1.21, 3.29, 0.29, 1.69, 1.71],
       [0.73, 3.22, 0.36, 1.55, 1.22]])
```

In this example, the first instance in `X_new` is located at a distance of about 2.81 from the first centroid, 0.33 from the second centroid, 2.90 from the third centroid, 1.49 from the fourth centroid, and 2.89 from the fifth centroid. If you have a high-dimensional dataset and you transform it this way, you end up with a *k*-dimensional dataset: this transformation can be a very efficient nonlinear dimensionality reduction technique. Alternatively, you can use these distances as extra features to train another model, as we did in Chapter 2.

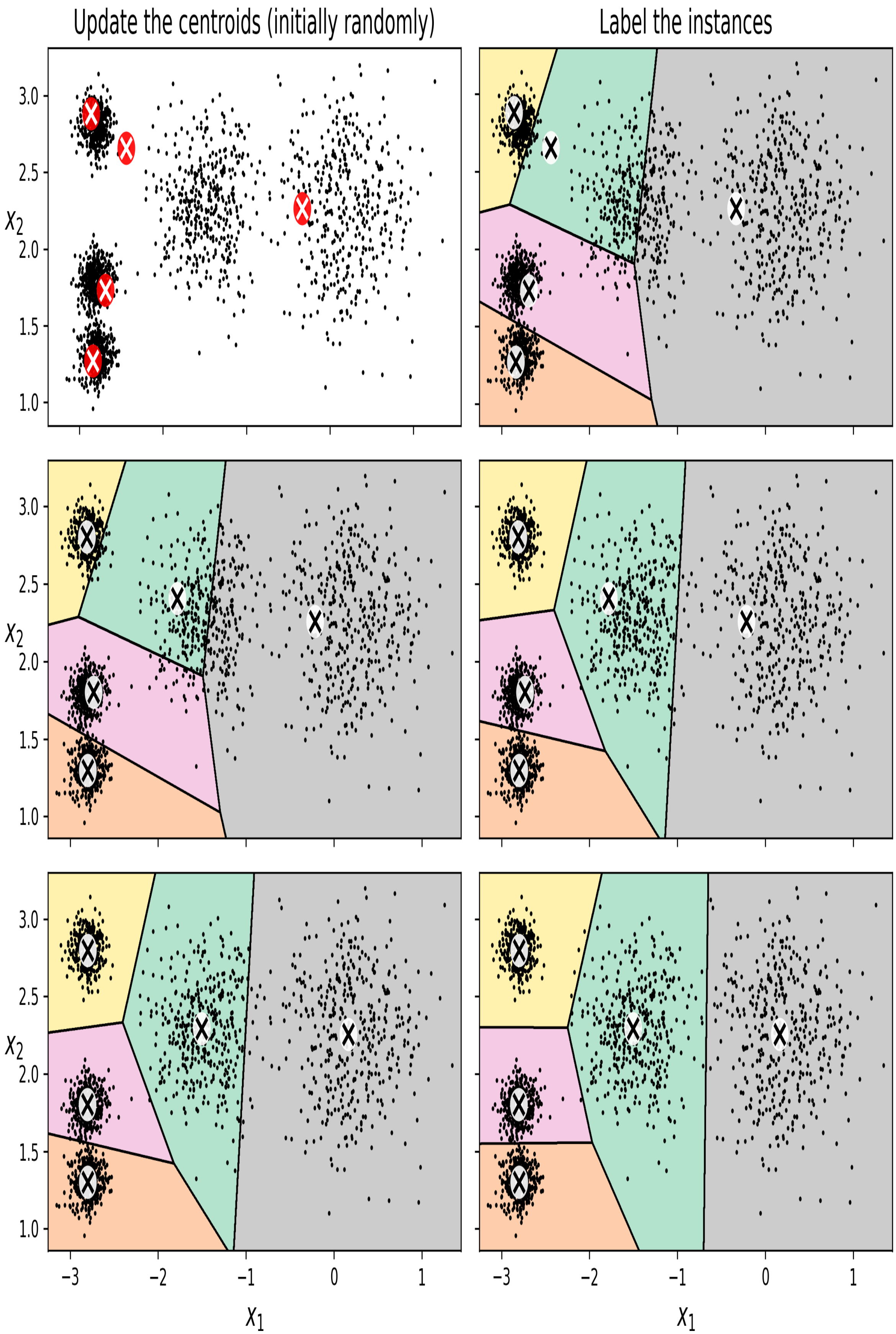
The K-Means algorithm

So, how does the algorithm work? Well, suppose you were given the centroids. You could easily label all the instances in the dataset by assigning each of them to the cluster whose centroid is closest. Conversely, if you were given all the instance labels, you could easily locate each cluster's centroid by computing the mean of the instances in that cluster. But you are given neither the labels nor the centroids, so how can you proceed? Well, just start by placing the centroids randomly (e.g., by picking *k* instances at random from the dataset and using their locations as centroids). Then label the instances, update the centroids, label the instances, update the centroids, and so on until the centroids stop moving. The algorithm is guaranteed to converge in a finite number of steps (usually quite small). That’s because the mean squared distance between the instances and their closest centroid can only go down at each step, and since it cannot be negative, it’s guaranteed to converge.

You can see the algorithm in action in Figure 9-4: the centroids are initialized randomly (top left), then the instances are labeled (top right), then the centroids are updated (center left), the instances are relabeled (center right), and so on. As you can see, in just three iterations, the algorithm has reached a clustering that seems close to optimal.

NOTE

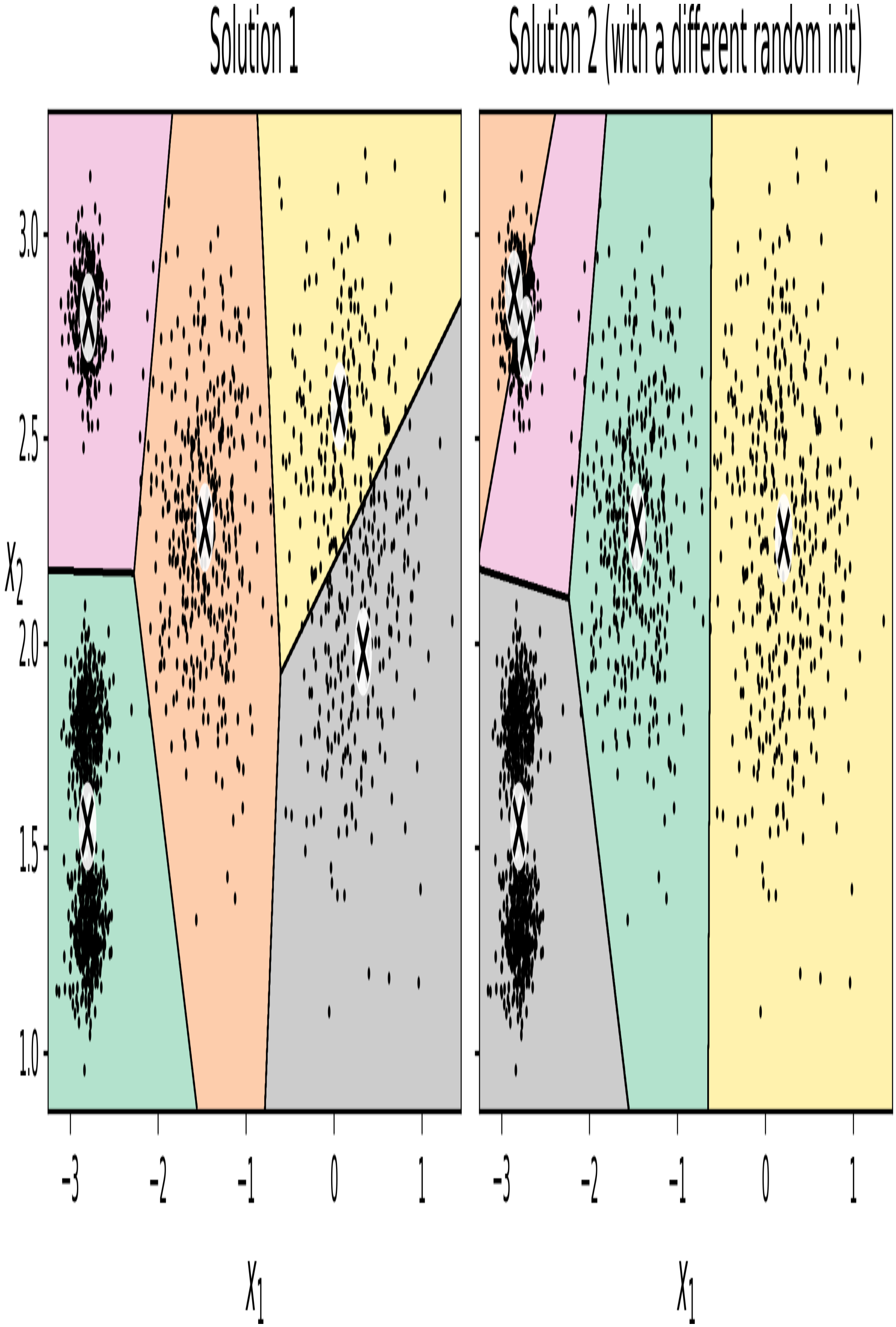
The computational complexity of the algorithm is generally linear with regard to the number of instances m, the number of clusters k, and the number of dimensions n. However, this is only true when the data has a clustering structure. If it does not, then in the worst-case scenario the complexity can increase exponentially with the number of instances. In practice, this rarely happens, and K-Means is generally one of the fastest clustering algorithms.



Update the centroids (initially randomly)
Label the instances
3.0
2.5
2.0
1.5
1.0
x_2
−3
−2
−1
0
1
x_1

Figure 9-4. The K-Means algorithm

Although the algorithm is guaranteed to converge, it may not converge to the right solution (i.e., it may converge to a local optimum): whether it does or not depends on the centroid initialization. Figure 9-5 shows two suboptimal solutions that the algorithm can converge to if you are not lucky with the random initialization step.



Solution 1
Solution 2 (with a different random init)
3.0
2.5
2.0
1.5
1.0
x_2
-3
-2
-1
0
1
x_1
x_1

Figure 9-5. Suboptimal solutions due to unlucky centroid initializations

Let’s look at a few ways you can mitigate this risk by improving the centroid initialization.

Centroid initialization methods

If you happen to know approximately where the centroids should be (e.g., if you ran another clustering algorithm earlier), then you can set the `init` hyperparameter to a NumPy array containing the list of centroids, and set `n_init` to `1`:

```
good_init = np.array([[-3, 3], [-3, 2], [-3, 1], [-1, 2], [0,
2]])
kmeans = KMeans(n_clusters=5, init=good_init, n_init=1,
random_state=42)
kmeans.fit(X)
```

Another solution is to run the algorithm multiple times with different random initializations and keep the best solution. The number of random initializations is controlled by the `n_init` hyperparameter: by default, it is equal to `10`, which means that the whole algorithm described earlier runs 10 times when you call `fit()`, and Scikit-Learn keeps the best solution. But how exactly does it know which solution is the best? It uses a performance metric! That metric is called the model’s *inertia*, which is the sum of the squared distances between the instances and their closest centroid. It is roughly equal to 219.4 for the model on the left in Figure 9-5, 258.6 for the model on the right in Figure 9-5, and only 211.6 for the model in Figure 9-3. The `KMeans` class runs the algorithm `n_init` times and keeps the model with the lowest inertia. In this example, the model in Figure 9-3 will be selected (unless we are very unlucky with `n_init` consecutive random initializations). If you are curious, a model’s inertia is accessible via the `inertia_` instance variable:

```
>>> kmeans.inertia_
211.59853725816836
```

The `score()` method returns the negative inertia. Why negative? Because a predictor's `score()` method must always respect Scikit-Learn's "greater is better" rule: if a predictor is better than another, its `score()` method should return a greater score.

```
>>> kmeans.score(X)
-211.5985372581684
```

An important improvement to the K-Means algorithm, *K-Means++*, was proposed in a 2006 paper by David Arthur and Sergei Vassilvitskii.[2] They introduced a smarter initialization step that tends to select centroids that are distant from one another, and this improvement makes the K-Means algorithm much less likely to converge to a suboptimal solution. They showed that the additional computation required for the smarter initialization step is well worth it because it makes it possible to drastically reduce the number of times the algorithm needs to be run to find the optimal solution. The K-Means++ initialization algorithm goes like this:

1. Take one centroid $\mathbf{c}^{(1)}$, chosen uniformly at random from the dataset.

2. Take a new centroid $\mathbf{c}^{(i)}$, choosing an instance $\mathbf{x}^{(i)}$ with probability $D\left(\mathbf{x}^{(i)}\right)^2 / \sum_{j=1}^{m} D\left(\mathbf{x}^{(j)}\right)^2$, where D($\mathbf{x}^{(i)}$) is the distance between the instance $\mathbf{x}^{(i)}$ and the closest centroid that was already chosen. This probability distribution ensures that instances farther away from already chosen centroids are much more likely be selected as centroids.

3. Repeat the previous step until all k centroids have been chosen.

The `KMeans` class uses this initialization method by default.

Accelerated K-Means and mini-batch K-Means

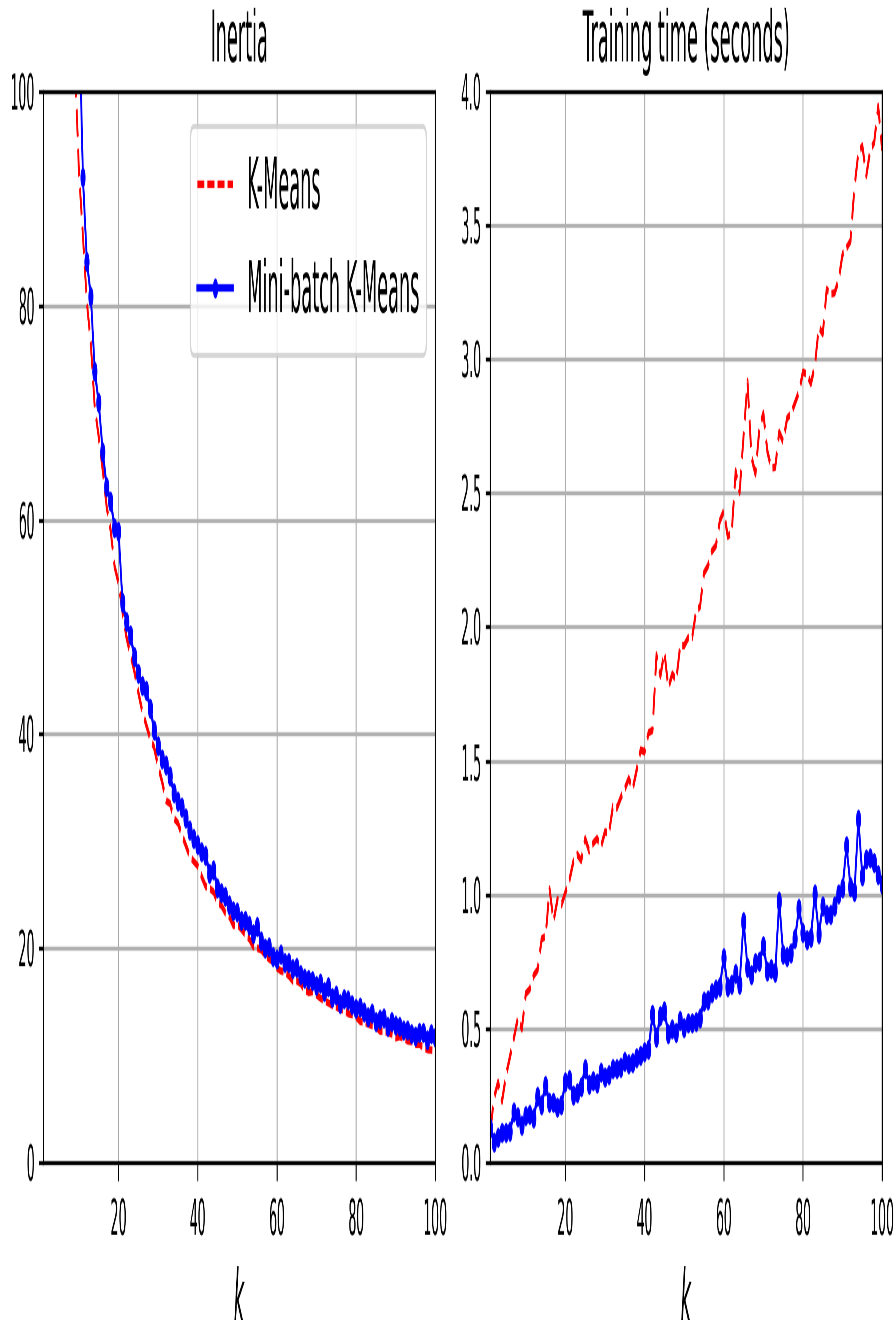
Another improvement to the K-Means algorithm was proposed in a 2003 paper by Charles Elkan.[3] On some large datasets with many clusters, it can accelerate the algorithm by avoiding many unnecessary distance calculations. Elkan achieved this by exploiting the triangle inequality (i.e., that a straight line is always the shortest distance between two points[4]) and by keeping track of lower and upper bounds for distances between instances and centroids. However, Elkan's algorithm does not always accelerate training, it depends on the dataset, and sometimes it can even slow down training significantly. Still, if you want to give it a try, set `algorithm="elkan"`.

Yet another important variant of the K-Means algorithm was proposed in a 2010 paper by David Sculley.[5] Instead of using the full dataset at each iteration, the algorithm is capable of using mini-batches, moving the centroids just slightly at each iteration. This speeds up the algorithm typically by a factor of three to four and makes it possible to cluster huge datasets that do not fit in memory. Scikit-Learn implements this algorithm in the `MiniBatchKMeans` class. You can just use this class like the `KMeans` class:

```
from sklearn.cluster import MiniBatchKMeans

minibatch_kmeans = MiniBatchKMeans(n_clusters=5, random_state=42)
minibatch_kmeans.fit(X)
```

If the dataset does not fit in memory, the simplest option is to use the `memmap` class, as we did for incremental PCA in Chapter 8. Alternatively, you can pass one mini-batch at a time to the `partial_fit()` method, but this will require much more work, since you will need to perform multiple initializations and select the best one yourself.

Although the Mini-batch K-Means algorithm is much faster than the regular K-Means algorithm, its inertia is generally slightly worse. You can see this in Figure 9-6: the plot on the left compares the inertias of Mini-batch K-Means and regular K-Means models trained on the previous five-blobs dataset using various numbers of clusters *k*. The difference between the two curves is small, but visible. In the plot on the right, you can see that Mini-batch K-Means is roughly 3.5 times faster than regular K-Means on this dataset.



Inertia
Training time (seconds)
K-Means
Mini-batch K-Means
100
80
60
40
20
0
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
20
40
60
80
100
k
k

Figure 9-6. Mini-batch K-Means has a higher inertia than K-Means (left) but it is much faster (right), especially as k increases

Finding the optimal number of clusters

So far, we have set the number of clusters *k* to 5 because it was obvious by looking at the data that this was the correct number of clusters. But in general, it will not be so easy to know how to set *k*, and the result might be quite bad if you set it to the wrong value. As you can see in Figure 9-7, setting *k* to 3 or 8 results in fairly bad models.

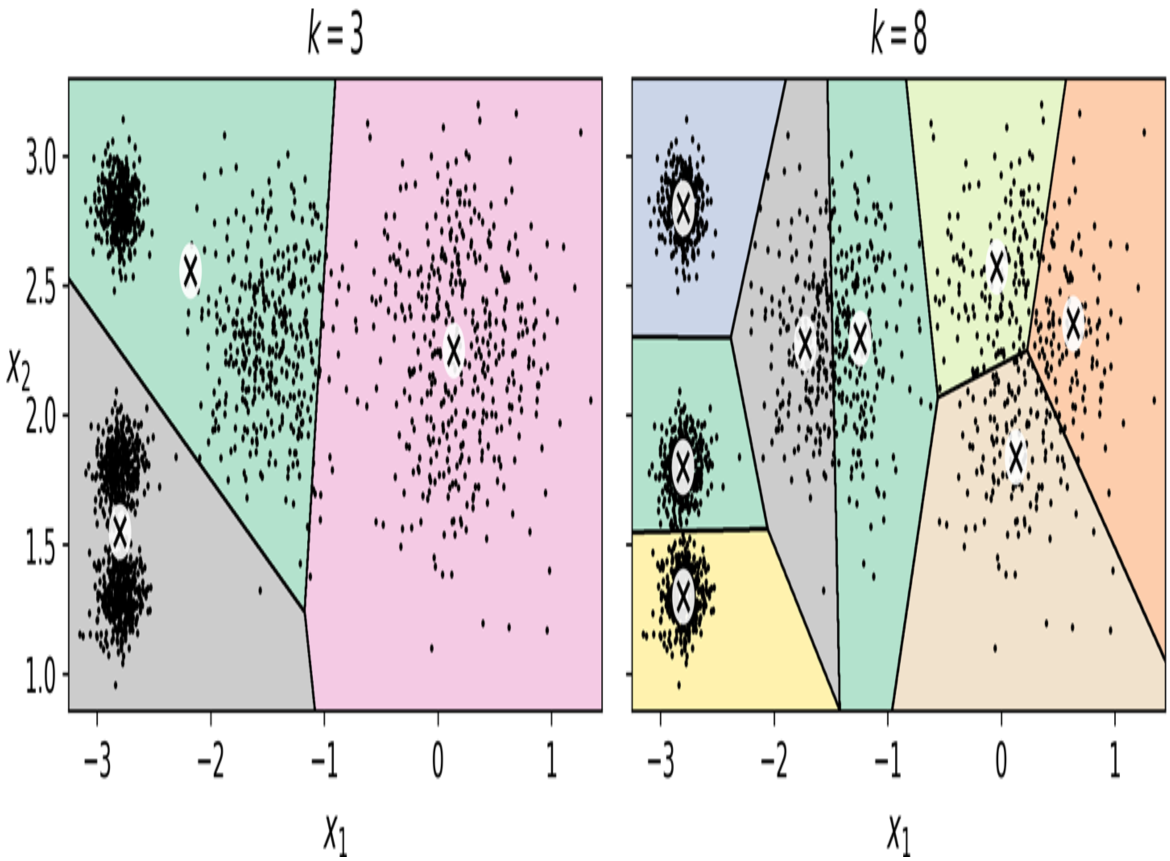


Figure 9-7. Bad choices for the number of clusters: when k is too small, separate clusters get merged (left), and when k is too large, some clusters get chopped into multiple pieces (right)

You might be thinking that we could just pick the model with the lowest inertia, right? Unfortunately, it is not that simple. The inertia for *k*=3 is about 653.2, which is much higher than for *k*=5 (which was 211.6). But with *k*=8, the inertia is just 119.1. The inertia is not a good performance metric when trying to choose *k* because it keeps getting lower as we increase *k*. Indeed, the more clusters there are, the closer each instance will be to its closest centroid, and therefore the lower the inertia will be. Let's plot the inertia as a function of *k* (see Figure 9-8).

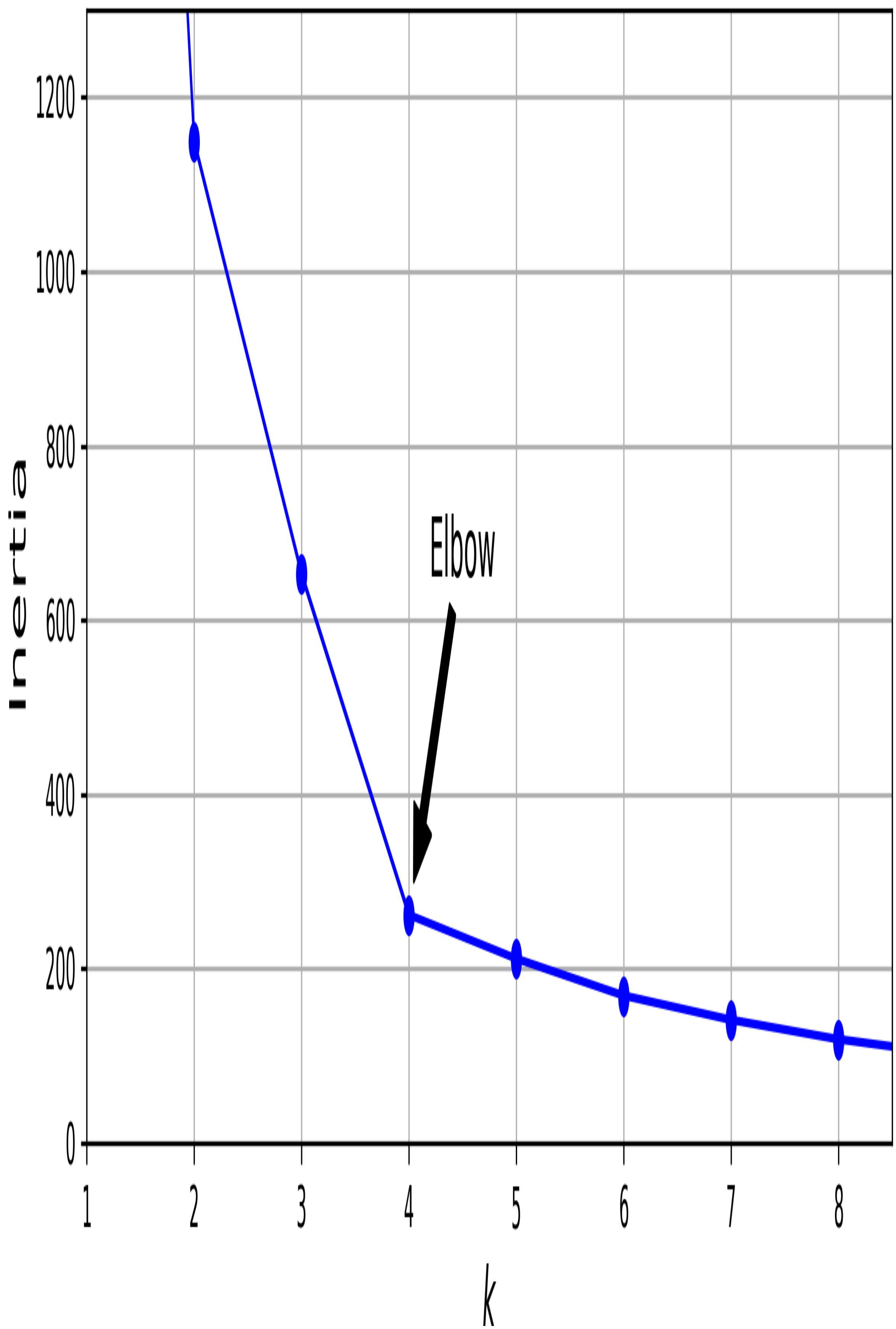

Inertia
1200
1000
800
600
400
200
0
Elbow
1
2
3
4
5
6
7
8
k

Figure 9-8. When plotting the inertia as a function of the number of clusters k, the curve often contains an inflexion point called the "elbow"

As you can see, the inertia drops very quickly as we increase k up to 4, but then it decreases much more slowly as we keep increasing k. This curve has roughly the shape of an arm, and there is an "elbow" at $k = 4$. So, if we did not know better, 4 would be a good choice: any lower value would be dramatic, while any higher value would not help much, and we might just be splitting perfectly good clusters in half for no good reason.

This technique for choosing the best value for the number of clusters is rather coarse. A more precise approach (but also more computationally expensive) is to use the *silhouette score*, which is the mean *silhouette coefficient* over all the instances. An instance's silhouette coefficient is equal to $(b – a) / \max(a, b)$, where a is the mean distance to the other instances in the same cluster (i.e., the mean intra-cluster distance) and b is the mean nearest-cluster distance (i.e., the mean distance to the instances of the next closest cluster, defined as the one that minimizes b, excluding the instance's own cluster). The silhouette coefficient can vary between –1 and +1. A coefficient close to +1 means that the instance is well inside its own cluster and far from other clusters, while a coefficient close to 0 means that it is close to a cluster boundary, and finally a coefficient close to –1 means that the instance may have been assigned to the wrong cluster.

To compute the silhouette score, you can use Scikit-Learn's `silhouette_score()` function, giving it all the instances in the dataset and the labels they were assigned:

```
>>> from sklearn.metrics import silhouette_score
>>> silhouette_score(X, kmeans.labels_)
0.655517642572828
```

Let's compare the silhouette scores for different numbers of clusters (see Figure 9-9).

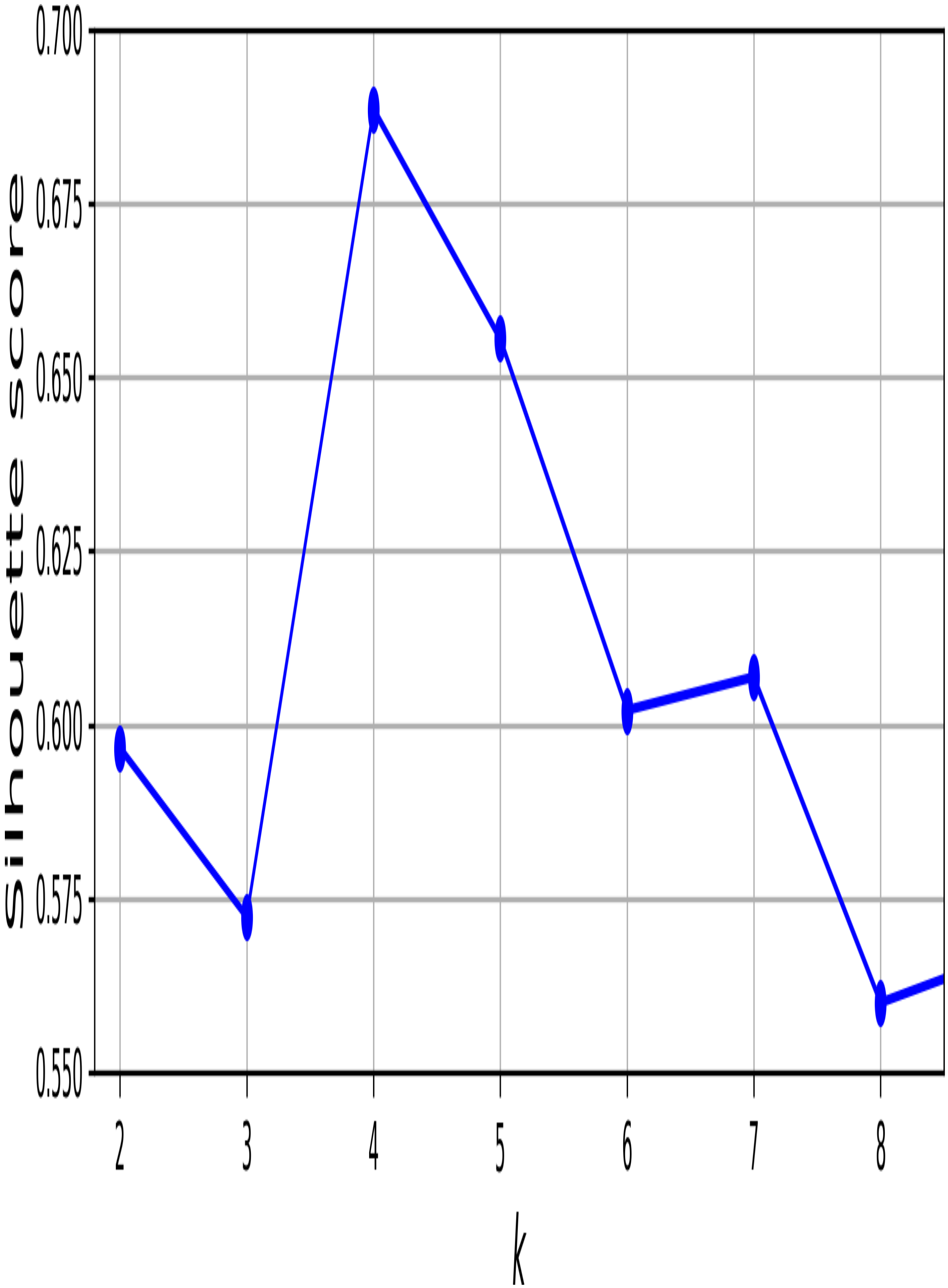
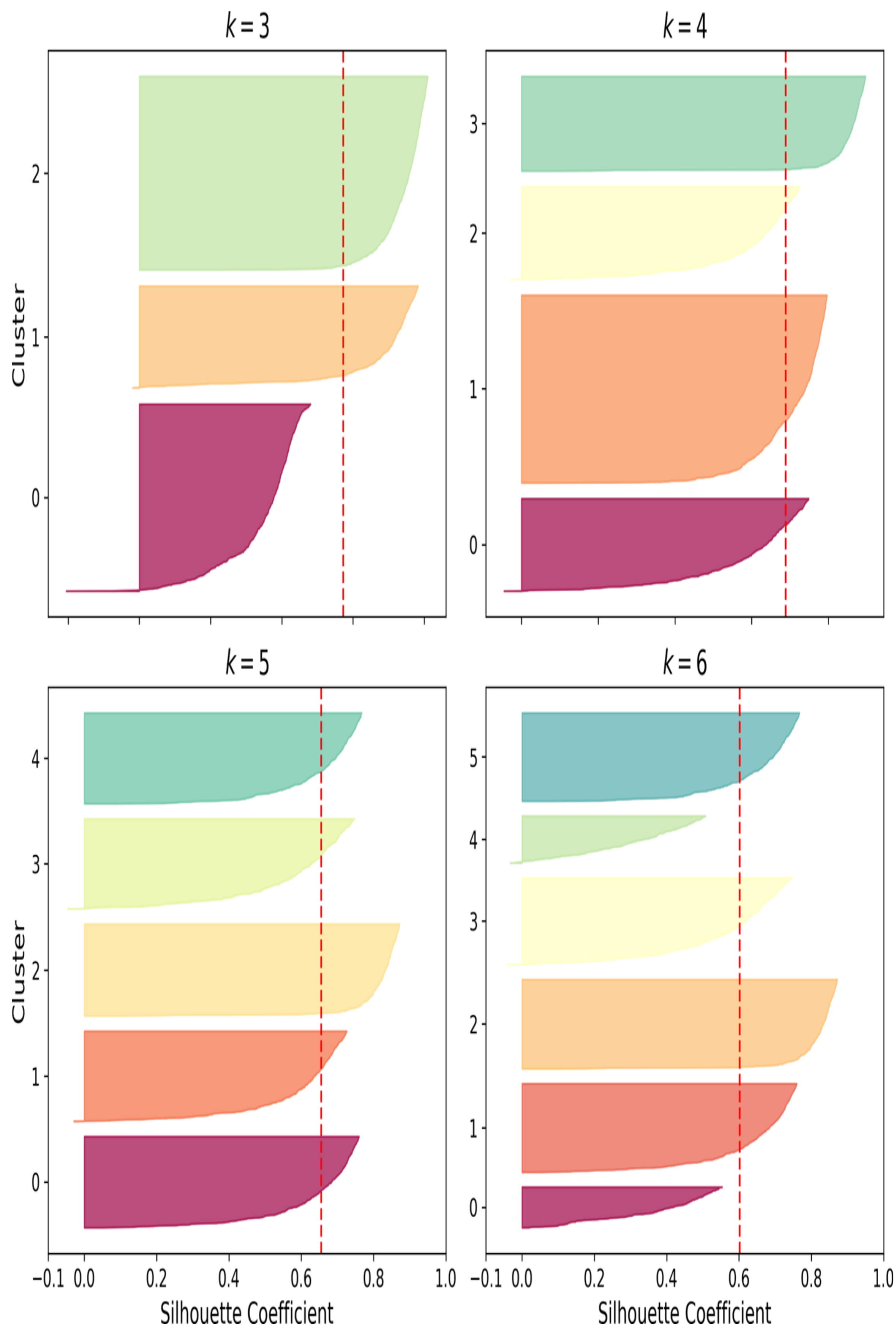


Figure 9-9. Selecting the number of clusters k using the silhouette score

As you can see, this visualization is much richer than the previous one: although it confirms that $k = 4$ is a very good choice, it also underlines the fact that $k = 5$ is quite good as well, and much better than $k = 6$ or 7. This was not visible when comparing inertias.

An even more informative visualization is obtained when you plot every instance's silhouette coefficient, sorted by the cluster they are assigned to and by the value of the coefficient. This is called a *silhouette diagram* (see Figure 9-10). Each diagram contains one knife shape per cluster. The shape's height indicates the number of instances in the cluster, and its width represents the sorted silhouette coefficients of the instances in the cluster (wider is better). The dashed line indicates the mean silhouette coefficient.



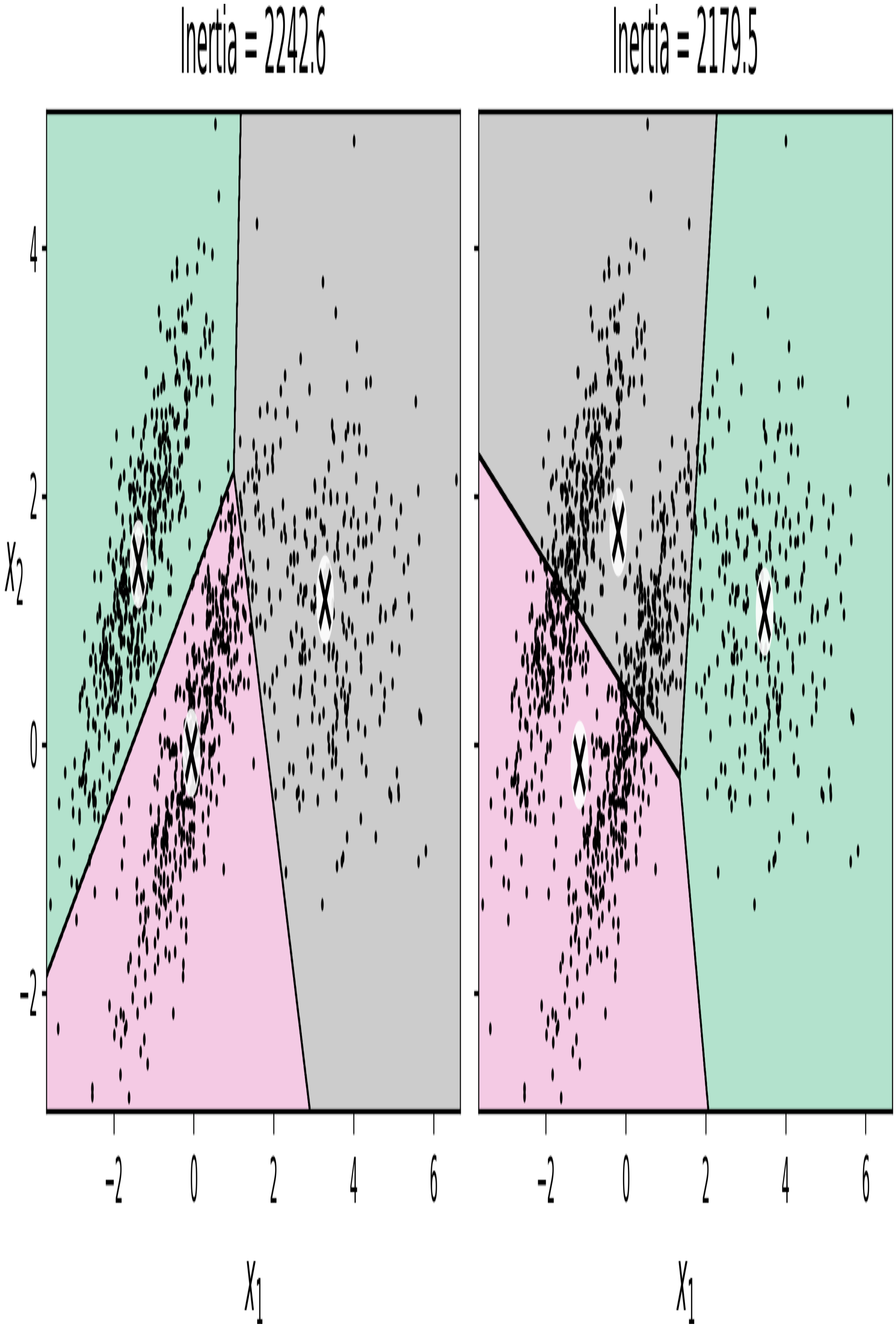
$k = 3$
$k = 4$
$k = 5$
$k = 6$
Cluster
Cluster
Silhouette Coefficient
Silhouette Coefficient
−0.1 0.0 0.2 0.4 0.6 0.8 1.0
−0.1 0.0 0.2 0.4 0.6 0.8 1.0

Figure 9-10. Analyzing the silhouette diagrams for various values of k

The vertical dashed lines represent the silhouette score for each number of clusters. When most of the instances in a cluster have a lower coefficient than this score (i.e., if many of the instances stop short of the dashed line, ending to the left of it), then the cluster is rather bad since this means its instances are much too close to other clusters. We can see that when $k = 3$ or 6, we get bad clusters. But when $k = 4$ or 5, the clusters look pretty good: most instances extend beyond the dashed line, to the right and closer to 1.0. When $k = 4$, the cluster at index 1 (the second from the bottom) is rather big. When $k = 5$, all clusters have similar sizes. So, even though the overall silhouette score from $k = 4$ is slightly greater than for $k = 5$, it seems like a good idea to use $k = 5$ to get clusters of similar sizes.

Limits of K-Means

Despite its many merits, most notably being fast and scalable, K-Means is not perfect. As we saw, it is necessary to run the algorithm several times to avoid suboptimal solutions, plus you need to specify the number of clusters, which can be quite a hassle. Moreover, K-Means does not behave very well when the clusters have varying sizes, different densities, or nonspherical shapes. For example, Figure 9-11 shows how K-Means clusters a dataset containing three ellipsoidal clusters of different dimensions, densities, and orientations.



Inertia = 2242.6
Inertia = 2179.5
x_2
4
2
0
-2
-2
0
2
4
6
x_1
x_1

Figure 9-11. K-Means fails to cluster these ellipsoidal blobs properly

As you can see, neither of these solutions is any good. The solution on the left is better, but it still chops off 25% of the middle cluster and assigns it to the cluster on the right. The solution on the right is just terrible, even though its inertia is lower. So, depending on the data, different clustering algorithms may perform better. On these types of elliptical clusters, Gaussian mixture models work great.

> **TIP**
>
> It is important to scale the input features before you run K-Means, or the clusters may be very stretched and K-Means will perform poorly. Scaling the features does not guarantee that all the clusters will be nice and spherical, but it generally helps K-Means.

Now let's look at a few ways we can benefit from clustering. We will use K-Means, but feel free to experiment with other clustering algorithms.

Using Clustering for Image Segmentation

Image segmentation is the task of partitioning an image into multiple segments. In *semantic segmentation*, all pixels that are part of the same object type get assigned to the same segment. For example, in a self-driving car's vision system, all pixels that are part of a pedestrian's image might be assigned to the "pedestrian" segment (there would be one segment containing all the pedestrians). In *instance segmentation*, all pixels that are part of the same individual object are assigned to the same segment. In this case there would be a different segment for each pedestrian. The state of the art in semantic or instance segmentation today is achieved using complex architectures based on convolutional neural networks (see Chapter 14). Here, we are going to do something much simpler: *color segmentation*. We will simply assign pixels to the same segment if they have a similar color. In some applications, this may be sufficient. For example, if you want to analyze satellite images to measure how much total forest area there is in a region, color segmentation may be just fine.

Let's use the Pillow package (Python Image Library) to load the *ladybug.png* image (see the upper-left image in Figure 9-12), assuming it's located at `filepath`:

```
>>> import PIL
>>> image = np.asarray(PIL.Image.open(filepath))
>>> image.shape
(533, 800, 3)
```

The image is represented as a 3D array. The first dimension's size is the height; the second is the width; and the third is the number of color channels, in this case red, green, and blue (RGB). In other words, for each pixel there is a 3D vector containing the intensities of red, green, and blue, as unsigned 8-bit integers between 0 and 255. Some images may have fewer channels, such as grayscale images (one channel). And some images may have more channels, such as images with an additional *alpha channel* for transparency, or satellite images which often contain channels for many light frequencies (e.g., infrared).

The following code reshapes the array to get a long list of RGB colors, then it clusters these colors using K-Means with 8 clusters, and it creates a `segmented_img` array containing the nearest cluster center for each pixel (i.e., the mean color of each pixel's cluster), and lastly it reshapes this array to the original image shape. The third line uses advanced NumPy indexing: for example, if the first 10 labels in `kmeans_.labels_` are equal to 1, then the first 10 colors in `segmented_img` are equal to `kmeans.cluster_centers_[1]`.

```
X = image.reshape(-1, 3)
kmeans = KMeans(n_clusters=8, random_state=42).fit(X)
segmented_img = kmeans.cluster_centers_[kmeans.labels_]
segmented_img = segmented_img.reshape(image.shape)
```

This outputs the image shown in the upper right of Figure 9-12. You can experiment with various numbers of clusters, as shown in the figure. When you use fewer than eight clusters, notice that the ladybug's flashy red color fails to get a cluster of its own: it gets merged with colors from the environment. This is because K-Means prefers clusters of similar sizes. The ladybug is small—much smaller than the rest of the image—so even though its color is flashy, K-Means fails to dedicate a cluster to it.


Original image
10 colors
8 colors
6 colors
4 colors
2 colors

Figure 9-12. Image segmentation using K-Means with various numbers of color clusters

That wasn't too hard, was it? Now let's look at another application of clustering.

Using Clustering for Semi-Supervised Learning

Another use case for clustering is in semi-supervised learning, when we have plenty of unlabeled instances and very few labeled instances. In this section, we'll use the digits dataset, which is a simple MNIST-like dataset containing 1,797 grayscale 8 × 8 images representing the digits 0 to 9. First, let's load and split the dataset (it's already shuffled):

```
from sklearn.datasets import load_digits

X_digits, y_digits = load_digits(return_X_y=True)
X_train, y_train = X_digits[:1400], y_digits[:1400]
X_test, y_test = X_digits[1400:], y_digits[1400:]
```

We will pretend we only have labels for 50 instances. To get a baseline performance, let's train a Logistic Regression model on these 50 labeled instances:

```
from sklearn.linear_model import LogisticRegression

n_labeled = 50
log_reg = LogisticRegression(max_iter=10_000)
log_reg.fit(X_train[:n_labeled], y_train[:n_labeled])
```

Let's measure the accuracy of this model on the test set (note that the test set must be labeled):

```
>>> log_reg.score(X_test, y_test)
0.7481108312342569
```

The model's accuracy is just 74.8%, while it would have reached 90.7% if we had trained it on the full training set. Let's see how we can do better. First, let's cluster the training set into 50 clusters. Then for each cluster, let’s find the image closest to the centroid. Let’s call these images the *representative images*:

```
k = 50
kmeans = KMeans(n_clusters=k, random_state=42)
X_digits_dist = kmeans.fit_transform(X_train)
representative_digit_idx = np.argmin(X_digits_dist, axis=0)
X_representative_digits = X_train[representative_digit_idx]
```

Figure 9-13 shows these 50 representative images.

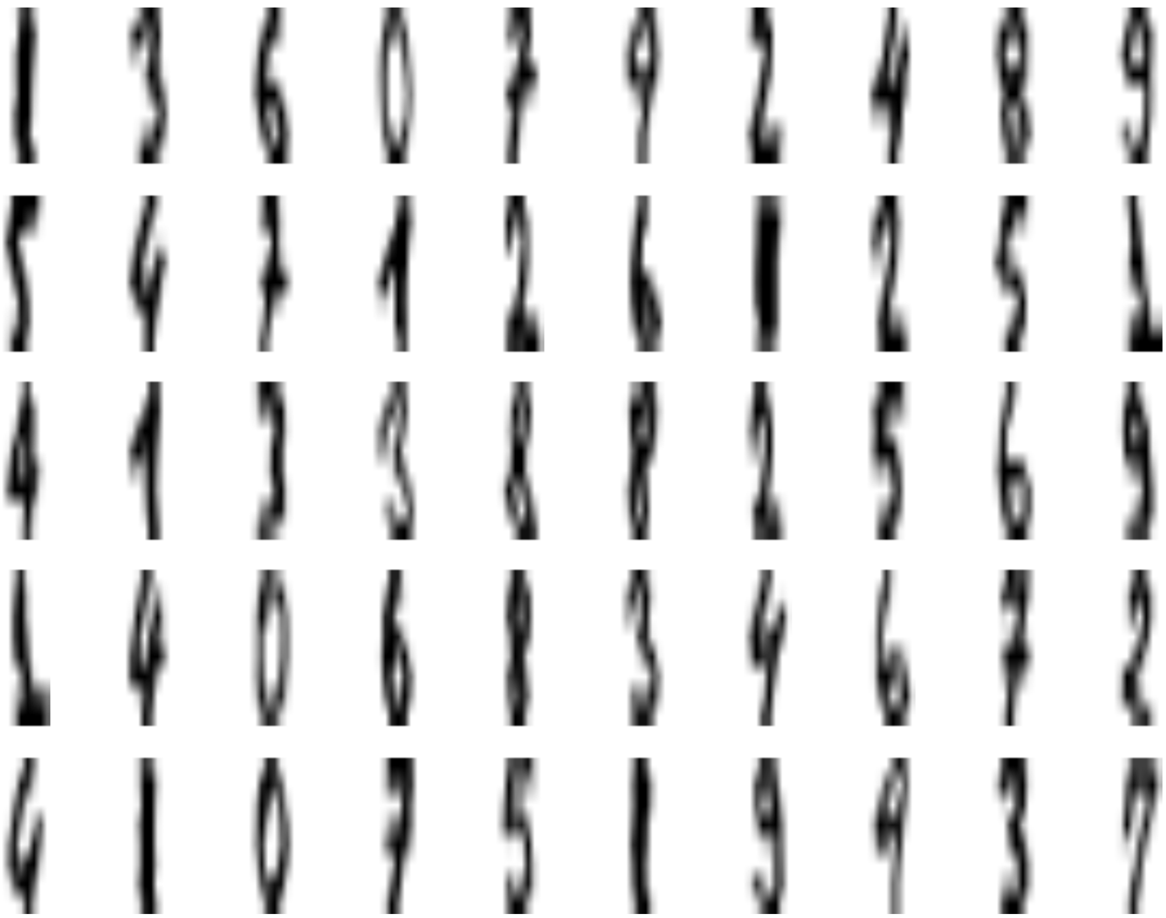


Figure 9-13. Fifty representative digit images (one per cluster)

Let’s look at each image and manually label it:

```
y_representative_digits = np.array([1, 3, 6, 0, 7, 9, 2, ..., 5,
1, 9, 9, 3, 7])
```

Now we have a dataset with just 50 labeled instances, but instead of being random instances, each of them is a representative image of its cluster. Let's see if the performance is any better:

```
>>> log_reg = LogisticRegression(max_iter=10_000)
>>> log_reg.fit(X_representative_digits, y_representative_digits)
>>> log_reg.score(X_test, y_test)
0.8488664987405542
```

Wow! We jumped from 74.8% accuracy to 84.9%, although we are still only training the model on 50 instances. Since it is often costly and painful to label instances, especially when it has to be done manually by experts, it is a good idea to label representative instances rather than just random instances.

But perhaps we can go one step further: what if we propagated the labels to all the other instances in the same cluster? This is called *label propagation*:

```
y_train_propagated = np.empty(len(X_train), dtype=np.int64)
for i in range(k):
    y_train_propagated[kmeans.labels_ == i] =
y_representative_digits[i]
```

Now let's train the model again and look at its performance:

```
>>> log_reg = LogisticRegression()
>>> log_reg.fit(X_train, y_train_propagated)
>>> log_reg.score(X_test, y_test)
0.8942065491183879
```

We got another significant accuracy boost! Let's see if we can do even better by ignoring the 1% instances that are farthest from their cluster center: this should eliminate some outliers. The following code first computes the distance from each instance to its closest cluster center, then for each cluster it sets the 1% largest distances to –1. Lastly, it creates a set without these instances marked with a –1 distance.

```
percentile_closest = 99
```

```
X_cluster_dist = X_digits_dist[np.arange(len(X_train)),
kmeans.labels_]
for i in range(k):
    in_cluster = (kmeans.labels_ == i)
    cluster_dist = X_cluster_dist[in_cluster]
    cutoff_distance = np.percentile(cluster_dist,
percentile_closest)
    above_cutoff = (X_cluster_dist > cutoff_distance)
    X_cluster_dist[in_cluster & above_cutoff] = -1

partially_propagated = (X_cluster_dist != -1)
X_train_partially_propagated = X_train[partially_propagated]
y_train_partially_propagated =
y_train_propagated[partially_propagated]
```

Now let's train the model again on this partially propagated dataset and see what accuracy we get:

```
>>> log_reg = LogisticRegression(max_iter=10_000)
>>> log_reg.fit(X_train_partially_propagated,
y_train_partially_propagated)
>>> log_reg.score(X_test, y_test)
0.9093198992443325
```

Nice! With just 50 labeled instances (only 5 examples per class on average!), we got 90.9% accuracy, which is actually very slightly higher than the performance we got on the fully labeled digits dataset (90.7%). This is partly thanks to the fact that we dropped some outliers, and partly because the propagated labels are actually pretty good—their accuracy is about 97.5%, as the following code shows:

```
>>> (y_train_partially_propagated ==
y_train[partially_propagated]).mean()
0.9755555555555555
```

TIP

Scikit-Learn also offers two classes that can propagate labels automatically: `LabelSpreading` and `LabelPropagation` in the `sklearn.semi_supervised` package. They both construct a similarity matrix between all the instances, and iteratively propagate labels from labeled instances to similar unlabeled instances. There's also a very different class called `SelfTrainingClassifier` in the same package: you give it a base classifier (such as a `RandomForestClassifier`) and it trains it on the labeled instances, then uses it to predict labels for the unlabeled samples. It then updates the training set with the labels it is most confident about. Lastly, it repeats this process of training and labeling until it cannot add labels anymore. These techniques are not magic bullets, but they can occasionally give your model a little boost.

ACTIVE LEARNING

To continue improving your model and your training set, the next step could be to do a few rounds of *active learning*, which is when a human expert interacts with the learning algorithm, providing labels for specific instances when the algorithm requests them. There are many different strategies for active learning, but one of the most common ones is called *uncertainty sampling*. Here is how it works:

1. The model is trained on the labeled instances gathered so far, and this model is used to make predictions on all the unlabeled instances.
2. The instances for which the model is most uncertain (i.e., when its estimated probability is lowest) are given to the expert for labeling.
3. You iterate this process until the performance improvement stops being worth the labeling effort.

Other active learning strategies include labeling the instances that would result in the largest model change, or the largest drop in the model's validation error, or the instances that different models disagree on (e.g., an SVM and a Random Forest).

Before we move on to Gaussian mixture models, let's take a look at DBSCAN, another popular clustering algorithm that illustrates a very different approach based on local density estimation. This approach allows the algorithm to identify clusters of arbitrary shapes.

DBSCAN

This algorithm defines clusters as continuous regions of high density. Here is how it works:

- For each instance, the algorithm counts how many instances are located within a small distance ε (epsilon) from it. This region is called the instance's *ε-neighborhood*.
- If an instance has at least `min_samples` instances in its ε-neighborhood (including itself), then it is considered a *core instance*. In other words, core instances are those that are located in dense regions.
- All instances in the neighborhood of a core instance belong to the same cluster. This neighborhood may include other core instances; therefore, a long sequence of neighboring core instances forms a single cluster.
- Any instance that is not a core instance and does not have one in its neighborhood is considered an anomaly.

This algorithm works well if all the clusters are well separated by low-density regions. The `DBSCAN` class in Scikit-Learn is as simple to use as you might expect. Let's test it on the moons dataset, introduced in Chapter 6:

```
from sklearn.cluster import DBSCAN
from sklearn.datasets import make_moons

X, y = make_moons(n_samples=1000, noise=0.05)
dbscan = DBSCAN(eps=0.05, min_samples=5)
dbscan.fit(X)
```

The labels of all the instances are now available in the `labels_` instance variable:

```
>>> dbscan.labels_
array([ 0,  2, -1, -1,  1,  0,  0,  0,  2,  5, [...], 3,  3,  4,
2,  6,  3])
```

Notice that some instances have a cluster index equal to –1, which means that they are considered as anomalies by the algorithm. The indices of the core instances are available in the `core_sample_indices_` instance variable, and the core instances themselves are available in the `components_` instance variable:

```
>>> dbscan.core_sample_indices_
array([  0,   4,   5,   6,   7,   8,  10,  11, [...], 993, 995,
997, 998, 999])
>>> dbscan.components_
array([[-0.02137124,  0.40618608],
       [-0.84192557,  0.53058695],
       [...],
       [ 0.79419406,  0.60777171]])
```

This clustering is represented in the lefthand plot of Figure 9-14. As you can see, it identified quite a lot of anomalies, plus seven different clusters. How disappointing! Fortunately, if we widen each instance's neighborhood by increasing `eps` to 0.2, we get the clustering on the right, which looks perfect. Let's continue with this model.

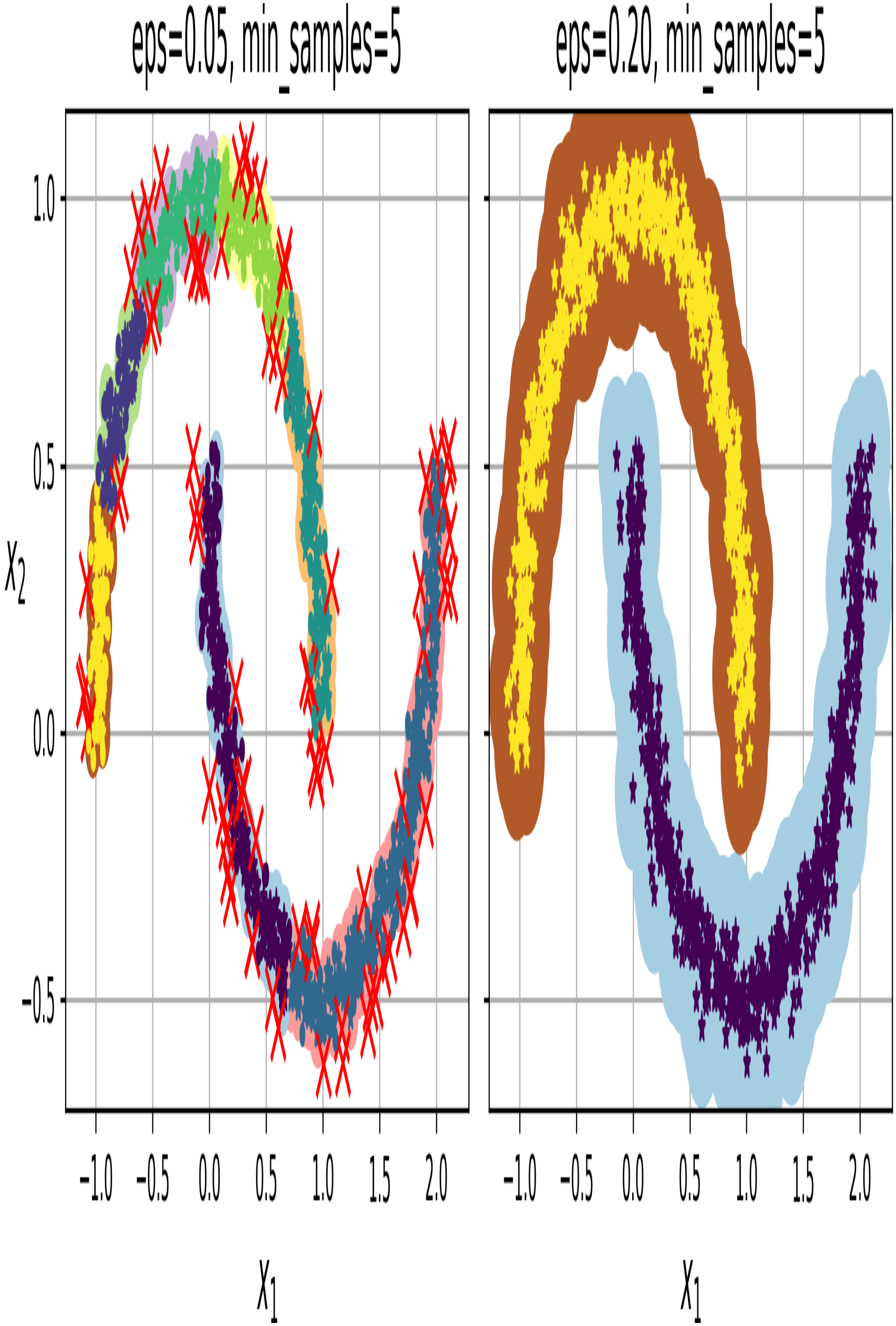

eps=0.05, min_samples=5
eps=0.20, min_samples=5
1.0
0.5
0.0
−0.5
x_2
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
x_1
x_1

Figure 9-14. DBSCAN clustering using two different neighborhood radiuses

Surprisingly, the `DBSCAN` class does not have a `predict()` method, although it has a `fit_predict()` method. In other words, it cannot predict which cluster a new instance belongs to. This decision was made because different classification algorithms can be better for different tasks, so the authors decided to let the user choose which one to use. Moreover, it's not hard to implement. For example, let's train a `KNeighborsClassifier`:

```
from sklearn.neighbors import KNeighborsClassifier

knn = KNeighborsClassifier(n_neighbors=50)
knn.fit(dbscan.components_,
dbscan.labels_[dbscan.core_sample_indices_])
```

Now, given a few new instances, we can predict which cluster they most likely belong to and even estimate a probability for each cluster:

```
>>> X_new = np.array([[-0.5, 0], [0, 0.5], [1, -0.1], [2, 1]])
>>> knn.predict(X_new)
array([1, 0, 1, 0])
>>> knn.predict_proba(X_new)
array([[0.18, 0.82],
       [1.  , 0.  ],
       [0.12, 0.88],
       [1.  , 0.  ]])
```

Note that we only trained the classifier on the core instances, but we could also have chosen to train it on all the instances, or all but the anomalies: this choice depends on the final task.

The decision boundary is represented in Figure 9-15 (the crosses represent the four instances in `X_new`). Notice that since there is no anomaly in the training set, the classifier always chooses a cluster, even when that cluster is far away. It is fairly straightforward to introduce a maximum distance, in which case the two instances that are far away from both clusters are classified as anomalies. To do this, use the `kneighbors()` method of the `KNeighborsClassifier`. Given a set of instances, it returns the distances and the indices of the *k* nearest neighbors in the training set (two matrices, each with *k* columns):

```
>>> y_dist, y_pred_idx = knn.kneighbors(X_new, n_neighbors=1)
>>> y_pred = dbscan.labels_[dbscan.core_sample_indices_]
[y_pred_idx]
>>> y_pred[y_dist > 0.2] = -1
>>> y_pred.ravel()
array([-1,  0,  1, -1])
```

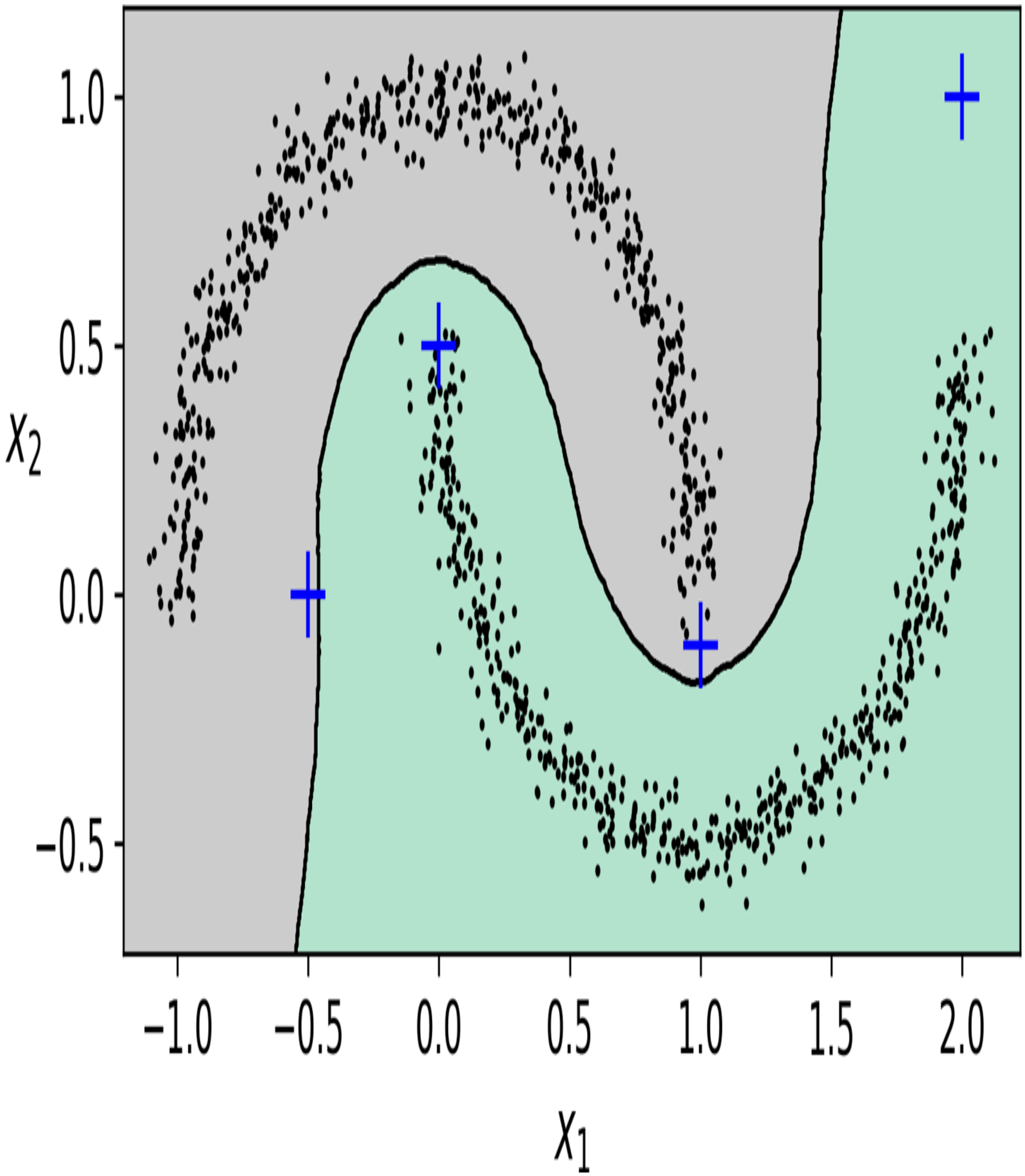


Figure 9-15. Decision boundary between two clusters

In short, DBSCAN is a very simple yet powerful algorithm capable of identifying any number of clusters of any shape. It is robust to outliers, and it has just two hyperparameters (`eps` and `min_samples`). If the density varies significantly across the clusters, or if there's no sufficiently low-density region around some clusters, DBSCAN can struggle to capture all the clusters properly. Moreover, its computational complexity is roughly ڽ□m_^{2}n), so it does not scale well to large datasets.

> **TIP**
>
> You may also want to try *Hierarchical DBSCAN* (HDBSCAN), which is implemented in the scikit-learn-contrib project.

Other Clustering Algorithms

Scikit-Learn implements several more clustering algorithms that you should take a look at. I cannot cover them all in detail here, but here is a brief overview:

Agglomerative clustering

A hierarchy of clusters is built from the bottom up. Think of many tiny bubbles floating on water and gradually attaching to each other until there's one big group of bubbles. Similarly, at each iteration, agglomerative clustering connects the nearest pair of clusters (starting with individual instances). If you drew a tree with a branch for every pair of clusters that merged, you would get a binary tree of clusters, where the leaves are the individual instances. This approach can capture clusters of various shapes, it also produces a flexible and informative cluster tree instead of forcing you to choose a particular cluster scale, and it can be used with any pairwise distance. It can scale nicely to large numbers of instances if you provide a connectivity matrix, which is a sparse $m \times m$ matrix that indicates which pairs of instances are neighbors (e.g., returned by `sklearn.neighbors.kneighbors_graph()`). Without a connectivity matrix, the algorithm does not scale well to large datasets.

BIRCH

The BIRCH (Balanced Iterative Reducing and Clustering using Hierarchies) algorithm was designed specifically for very large datasets, and it can be faster than batch K-Means, with similar results, as long as the number of features is not too large (<20). During training, it builds a tree structure containing just enough information to quickly assign each new instance to a cluster, without having to store all the instances in the tree: this approach allows it to use limited memory, while handling huge datasets.

Mean-Shift

This algorithm starts by placing a circle centered on each instance; then for each circle it computes the mean of all the instances located within it, and it shifts the circle so that it is centered on the mean. Next, it iterates this mean-shifting step until all the circles stop moving (i.e., until each of them is centered on the mean of the instances it contains). Mean-Shift shifts the circles in the direction of higher density, until each of them has found a local density maximum. Finally, all the instances whose circles have settled in the same place (or close enough) are assigned to the same cluster. Mean-Shift has some of the same features as DBSCAN, like how it can find any number of clusters of any shape, it has very few hyperparameters (just one—the radius of the circles, called the *bandwidth*), and it relies on local density estimation. But unlike DBSCAN, Mean-Shift tends to chop clusters into pieces when they have internal density variations. Unfortunately, its computational complexity is پ□m_^{2}n), so it is not suited for large datasets.

Affinity propagation

In this algorithm, instances repeatedly exchange messages between one another until every instance has elected another instance (or itself) to represent it. These elected instances are called *exemplars*. Each exemplar and all the instances that elected it form one cluster. In real-life politics, you typically want to vote for a candidate whose opinions are similar to yours, but you also want them to win the election, so you might choose a candidate you don't fully agree with, but who is more popular. You typically evaluate popularity through polls. Affinity propagation works in a similar way, and it tends to choose exemplars located near the center of clusters, similar to K-Means. But unlike with K-Means, you don’t have to pick a number of clusters ahead of time: it is determined during training. Moreover, affinity propagation can deal nicely with clusters of different sizes. Sadly, this algorithm has a computational complexity of ݑ□m_^{2}), so it is not suited for large datasets.

Spectral clustering

This algorithm takes a similarity matrix between the instances and creates a low-dimensional embedding from it (i.e., it reduces the matrix’s dimensionality), then it uses another clustering algorithm in this low-dimensional space (Scikit-Learn’s implementation uses K-Means). Spectral clustering can capture complex cluster structures, and it can also be used to cut graphs (e.g., to identify clusters of friends on a social network). It does not scale well to large numbers of instances, and it does not behave well when the clusters have very different sizes.

Now let’s dive into Gaussian mixture models, which can be used for density estimation, clustering, and anomaly detection.

Gaussian Mixtures

A *Gaussian mixture model* (GMM) is a probabilistic model that assumes that the instances were generated from a mixture of several Gaussian distributions whose parameters are unknown. All the instances generated from a single Gaussian distribution form a cluster that typically looks like an ellipsoid. Each cluster can have a different ellipsoidal shape, size, density, and orientation, just like in Figure 9-11. When you observe an instance, you know it was generated from one of the Gaussian distributions, but you are not told which one, and you do not know what the parameters of these distributions are.

There are several GMM variants. In the simplest variant, implemented in the `GaussianMixture` class, you must know in advance the number *k* of

Gaussian distributions. The dataset **X** is assumed to have been generated through the following probabilistic process:

- For each instance, a cluster is picked randomly from among k clusters. The probability of choosing the j^{th} cluster is the cluster's weight $\phi^{(j)}$.[6] The index of the cluster chosen for the i^{th} instance is noted $z^{(i)}$.

- If the i^{th} instance was assigned to the j^{th} cluster (i.e., $z^{(i)} = j$), then the location $\mathbf{x}^{(i)}$ of this instance is sampled randomly from the Gaussian distribution with mean $\boldsymbol{\mu}^{(j)}$ and covariance matrix $\boldsymbol{\Sigma}^{(j)}$. This is noted $\mathbf{x}^{(i)} \sim$ پ駿$\boldsymbol{\mu}^{(j)}$, *$\boldsymbol{\Sigma}^{(j)}$).

So, what can you do with such a model? Well, given the dataset **X**, you typically want to start by estimating the weights $\boldsymbol{\phi}$ and all the distribution parameters $\boldsymbol{\mu}^{(1)}$ to $\boldsymbol{\mu}^{(k)}$ and $\boldsymbol{\Sigma}^{(1)}$ to $\boldsymbol{\Sigma}^{(k)}$. Scikit-Learn's `GaussianMixture` class makes this super easy:

```
from sklearn.mixture import GaussianMixture

gm = GaussianMixture(n_components=3, n_init=10)
gm.fit(X)
```

Let's look at the parameters that the algorithm estimated:

```
>>> gm.weights_
array([0.39025715, 0.40007391, 0.20966893])
>>> gm.means_
array([[ 0.05131611,  0.07521837],
       [-1.40763156,  1.42708225],
       [ 3.39893794,  1.05928897]])
>>> gm.covariances_
array([[[ 0.68799922,  0.79606357],
        [ 0.79606357,  1.21236106]],

       [[ 0.63479409,  0.72970799],
        [ 0.72970799,  1.1610351 ]],

       [[ 1.14833585, -0.03256179],
        [-0.03256179,  0.95490931]]])
```

Great, it worked fine! Indeed, two of the three clusters were generated with 500 instances each, while the third cluster only contains 250 instances. So the true cluster weights are 0.4, 0.4, and 0.2, respectively, and that's roughly what the algorithm found. Similarly, the true means and covariance matrices are quite close to those found by the algorithm. But how? This class relies on the *Expectation-Maximization* (EM) algorithm, which has many similarities with the K-Means algorithm: it also initializes the cluster parameters randomly, then it repeats two steps until convergence, first assigning instances to clusters (this is called the *expectation step*) and then updating the clusters (this is called the *maximization step*). Sounds familiar, right? In the context of clustering, you can think of EM as a generalization of K-Means that not only finds the cluster centers ($\mathbf{\mu}^{(1)}$ to $\mathbf{\mu}^{(k)}$), but also their size, shape, and orientation ($\mathbf{\Sigma}^{(1)}$ to $\mathbf{\Sigma}^{(k)}$), as well as their relative weights ($\phi^{(1)}$ to $\phi^{(k)}$). Unlike K-Means, though, EM uses soft cluster assignments, not hard assignments. For each instance, during the expectation step, the algorithm estimates the probability that it belongs to each cluster (based on the current cluster parameters). Then, during the maximization step, each cluster is updated using *all* the instances in the dataset, with each instance weighted by the estimated probability that it belongs to that cluster. These probabilities are called the *responsibilities* of the clusters for the instances. During the maximization step, each cluster's update will mostly be impacted by the instances it is most responsible for.

WARNING

Unfortunately, just like K-Means, EM can end up converging to poor solutions, so it needs to be run several times, keeping only the best solution. This is why we set `n_init` to `10`. Be careful: by default `n_init` is set to `1`.

You can check whether or not the algorithm converged and how many iterations it took:

```
>>> gm.converged_
True
```

```
>>> gm.n_iter_
4
```

Now that you have an estimate of the location, size, shape, orientation, and relative weight of each cluster, the model can easily assign each instance to the most likely cluster (hard clustering) or estimate the probability that it belongs to a particular cluster (soft clustering). Just use the `predict()` method for hard clustering, or the `predict_proba()` method for soft clustering:

```
>>> gm.predict(X)
array([0, 0, 1, ..., 2, 2, 2])
>>> gm.predict_proba(X).round(3)
array([[0.977, 0.   , 0.023],
       [0.983, 0.001, 0.016],
       [0.   , 1.   , 0.   ],
       ...,
       [0.   , 0.   , 1.   ],
       [0.   , 0.   , 1.   ],
       [0.   , 0.   , 1.   ]])
```

A Gaussian mixture model is a *generative model*, meaning you can sample new instances from it (note that they are ordered by cluster index):

```
>>> X_new, y_new = gm.sample(6)
>>> X_new
array([[-0.86944074, -0.32767626],
       [ 0.29836051,  0.28297011],
       [-2.8014927 , -0.09047309],
       [ 3.98203732,  1.49951491],
       [ 3.81677148,  0.53095244],
       [ 2.84104923, -0.73858639]])
>>> y_new
array([0, 0, 1, 2, 2, 2])
```

It is also possible to estimate the density of the model at any given location. This is achieved using the `score_samples()` method: for each instance it is given, this method estimates the log of the *probability density function* (PDF) at that location. The greater the score, the higher the density:

```
>>> gm.score_samples(X).round(2)
array([-2.61, -3.57, -3.33, ..., -3.51, -4.4 , -3.81])
```

If you compute the exponential of these scores, you get the value of the PDF at the location of the given instances. These are not probabilities, but probability *densities*: they can take on any positive value, not just a value between 0 and 1. To estimate the probability that an instance will fall within a particular region, you would have to integrate the PDF over that region (if you do so over the entire space of possible instance locations, the result will be 1).

Figure 9-16 shows the cluster means, the decision boundaries (dashed lines), and the density contours of this model.

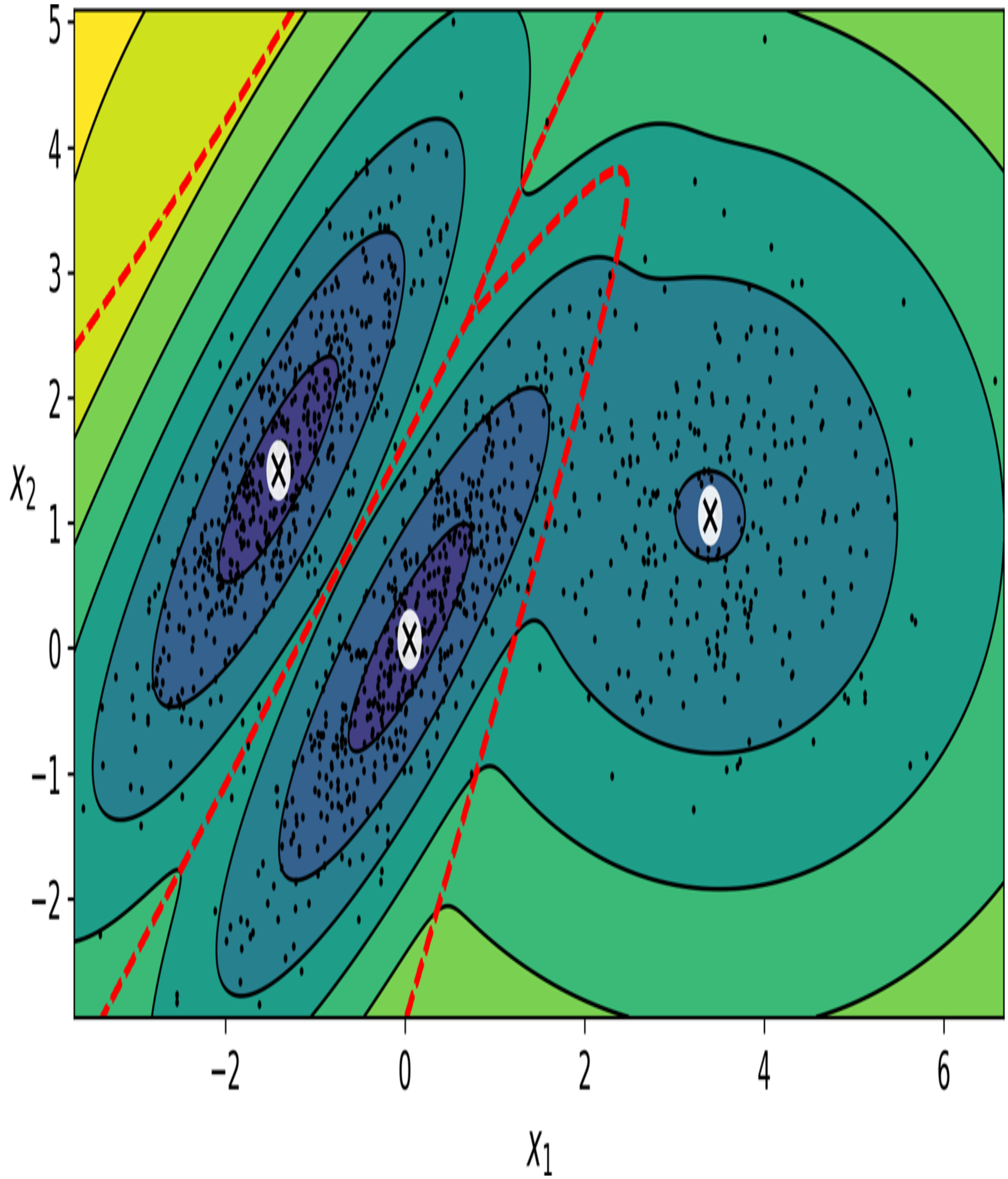


Figure 9-16. Cluster means, decision boundaries, and density contours of a trained Gaussian mixture model

Nice! The algorithm clearly found an excellent solution. Of course, we made its task easy by generating the data using a set of 2D Gaussian distributions (unfortunately, real-life data is not always so Gaussian and low-dimensional). We also gave the algorithm the correct number of clusters. When there are many dimensions, or many clusters, or few instances, EM can struggle to converge to the optimal solution. You might need to reduce the difficulty of the task by limiting the number of parameters that the algorithm has to learn. One way to do this is to limit the range of shapes and orientations that the clusters can have. This can be achieved by imposing constraints on the covariance matrices. To do this, set the `covariance_type` hyperparameter to one of the following values:

`"spherical"`

All clusters must be spherical, but they can have different diameters (i.e., different variances).

`"diag"`

Clusters can take on any ellipsoidal shape of any size, but the ellipsoid's axes must be parallel to the coordinate axes (i.e., the covariance matrices must be diagonal).

`"tied"`

All clusters must have the same ellipsoidal shape, size, and orientation (i.e., all clusters share the same covariance matrix).

By default, `covariance_type` is equal to `"full"`, which means that each cluster can take on any shape, size, and orientation (it has its own unconstrained covariance matrix). Figure 9-17 plots the solutions found by the EM algorithm when `covariance_type` is set to `"tied"` or `"spherical`."

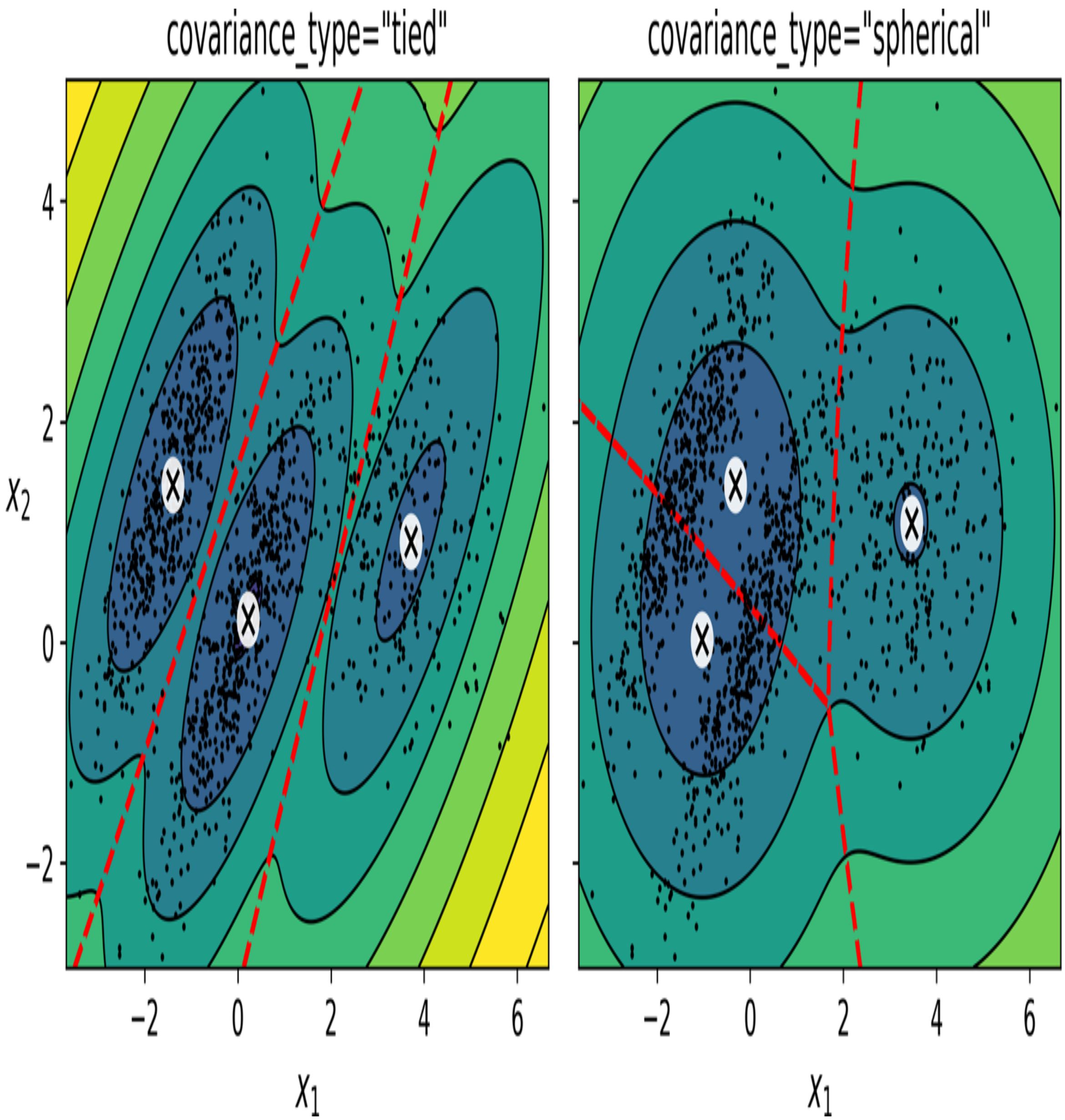


Figure 9-17. Gaussian mixtures for tied clusters (left) and spherical clusters (right)

NOTE

The computational complexity of training a `GaussianMixture` model depends on the number of instances *m*, the number of dimensions *n*, the number of clusters *k*, and the constraints on the covariance matrices. If `covariance_type` is `"spherical` or `"diag"`, it is ﭘ□kmn_), assuming the data has a clustering structure. If `covariance_type` is `"tied"` or `"full"`, it is ﭘ□kmn_^{2} + kn^3), so it will not scale to large numbers of features.

Gaussian mixture models can also be used for anomaly detection. Let's see how.

Anomaly Detection Using Gaussian Mixtures

Anomaly detection (also called *outlier detection*) is the task of detecting instances that deviate strongly from the norm. These instances are called *anomalies*, or *outliers*, while the normal instances are called *inliers*. Anomaly detection is useful in a wide variety of applications, such as fraud detection, detecting defective products in manufacturing, or removing outliers from a dataset before training another model, which can significantly improve the performance of the resulting model.

Using a Gaussian mixture model for anomaly detection is quite simple: any instance located in a low-density region can be considered an anomaly. You must define what density threshold you want to use. For example, in a manufacturing company that tries to detect defective products, the ratio of defective products is usually well known. Say it is equal to 2%. You then set the density threshold to be the value that results in having 2% of the instances located in areas below that threshold density. If you notice that you get too many false positives (i.e., perfectly good products that are flagged as defective), you can lower the threshold. Conversely, if you have too many false negatives (i.e., defective products that the system does not flag as defective), you can increase the threshold. This is the usual precision/recall trade-off (see Chapter 3). Here is how you would identify the outliers using the fourth percentile lowest density as the threshold (i.e., approximately 4% of the instances will be flagged as anomalies):

```
densities = gm.score_samples(X)
density_threshold = np.percentile(densities, 2)
anomalies = X[densities < density_threshold]
```

Figure 9-18 represents these anomalies as stars.

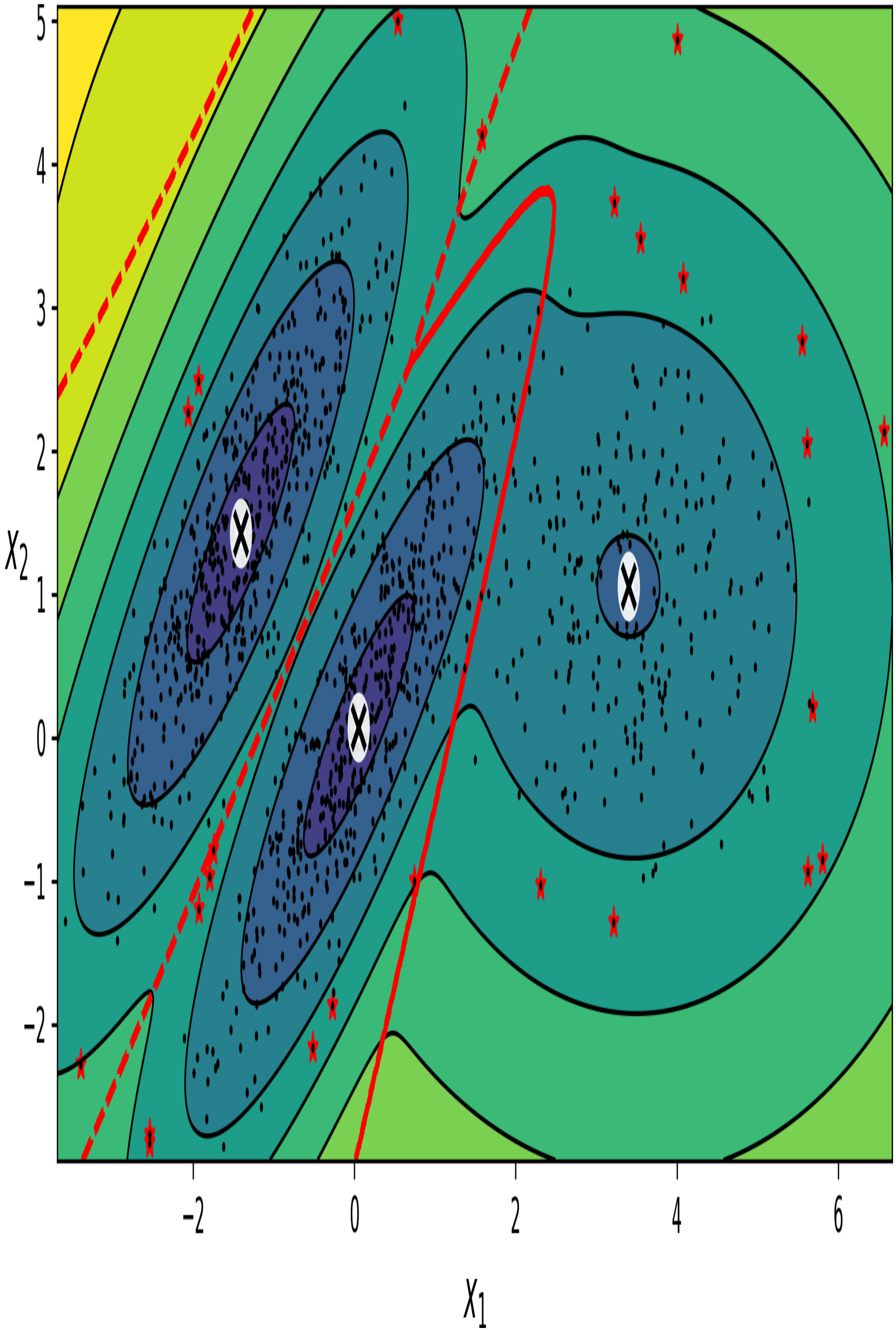

5
4
3
2
1
0
-1
-2
-2
0
2
4
6
x_1
x_2

Figure 9-18. Anomaly detection using a Gaussian mixture model

A closely related task is *novelty detection*: it differs from anomaly detection in that the algorithm is assumed to be trained on a "clean" dataset, uncontaminated by outliers, whereas anomaly detection does not make this assumption. Indeed, outlier detection is often used to clean up a dataset.

> **TIP**
>
> Gaussian mixture models try to fit all the data, including the outliers, so if you have too many of them, this will bias the model's view of "normality," and some outliers may wrongly be considered as normal. If this happens, you can try to fit the model once, use it to detect and remove the most extreme outliers, then fit the model again on the cleaned-up dataset. Another approach is to use robust covariance estimation methods (see the `EllipticEnvelope` class).

Just like K-Means, the `GaussianMixture` algorithm requires you to specify the number of clusters. So, how can you find it?

Selecting the Number of Clusters

With K-Means, you could use the inertia or the silhouette score to select the appropriate number of clusters. But with Gaussian mixtures, it is not possible to use these metrics because they are not reliable when the clusters are not spherical or have different sizes. Instead, you can try to find the model that minimizes a *theoretical information criterion*, such as the *Bayesian information criterion* (BIC) or the *Akaike information criterion* (AIC), defined in Equation 9-1.

Equation 9-1. Bayesian information criterion (BIC) and Akaike information criterion (AIC)

$$
\begin{aligned}
BIC &= \log(m)p - 2\log\left(\widehat{\mathscr{L}}\right) \\
AIC &= 2p - 2\log\left(\widehat{\mathscr{L}}\right)
\end{aligned}
$$

In these equations:

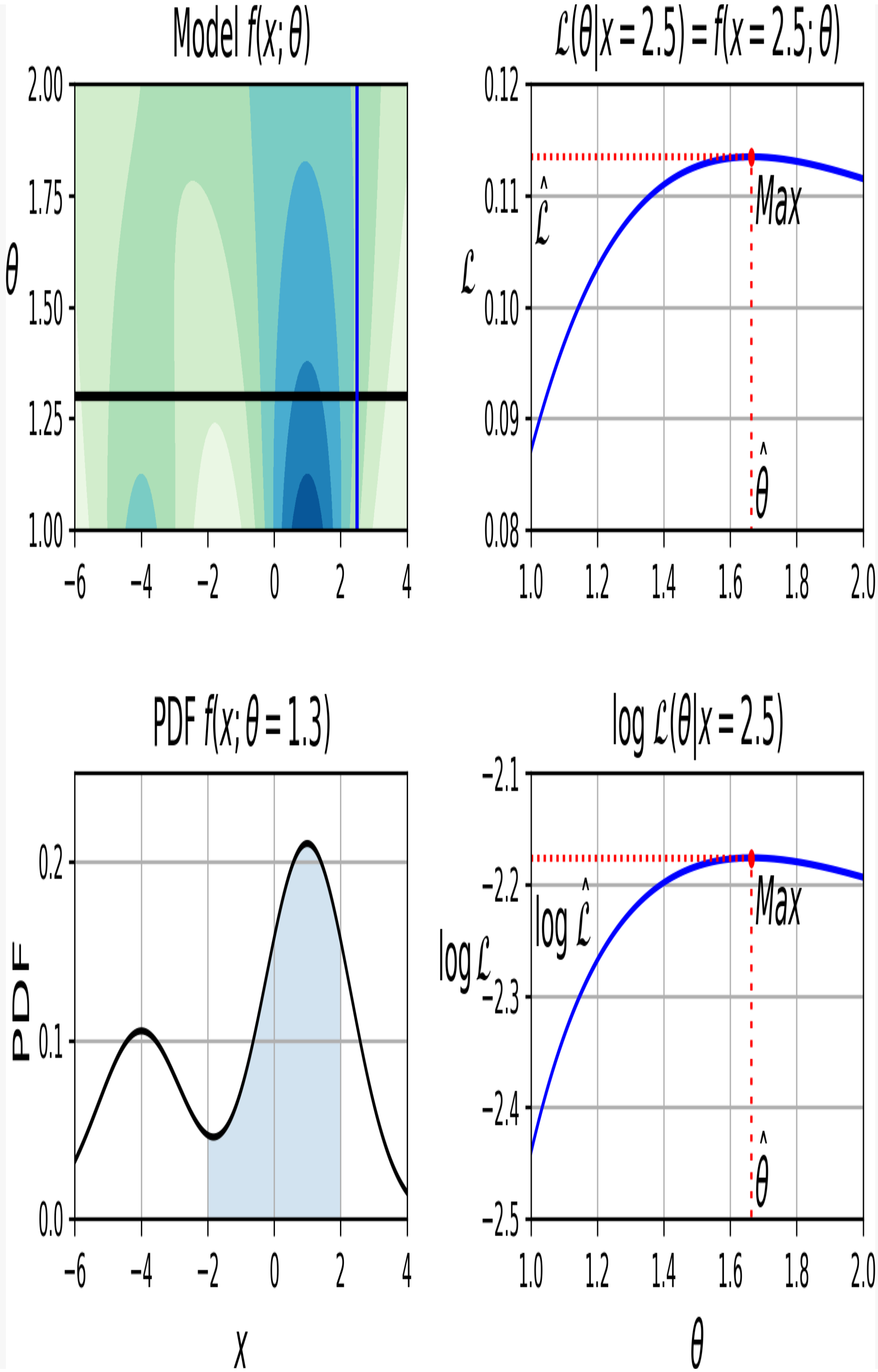
- m is the number of instances, as always.
- p is the number of parameters learned by the model.
- $\widehat{\mathscr{L}}$ is the maximized value of the *likelihood function* of the model.

Both the BIC and the AIC penalize models that have more parameters to learn (e.g., more clusters) and reward models that fit the data well. They often end up selecting the same model. When they differ, the model selected by the BIC tends to be simpler (fewer parameters) than the one selected by the AIC, but tends to not fit the data quite as well (this is especially true for larger datasets).

LIKELIHOOD FUNCTION

The terms "probability" and "likelihood" are often used interchangeably in everyday language, but they have very different meanings in statistics. Given a statistical model with some parameters $\boldsymbol{\theta}$, the word "probability" is used to describe how plausible a future outcome $\mathbf{x}$ is (knowing the parameter values $\boldsymbol{\theta}$), while the word "likelihood" is used to describe how plausible a particular set of parameter values $\boldsymbol{\theta}$ are, after the outcome $\mathbf{x}$ is known.

Consider a 1D mixture model of two Gaussian distributions centered at –4 and +1. For simplicity, this toy model has a single parameter θ that controls the standard deviations of both distributions. The top-left contour plot in Figure 9-19 shows the entire model $f(x; \theta)$ as a function of both x and θ. To estimate the probability distribution of a future outcome x, you need to set the model parameter θ. For example, if you set θ to 1.3 (the horizontal line), you get the probability density function $f(x; \theta=1.3)$ shown in the lower-left plot. Say you want to estimate the probability that x will fall between –2 and +2. You must calculate the integral of the PDF on this range (i.e., the surface of the shaded region). But what if you don't know θ, and instead if you have observed a single instance $x=2.5$ (the vertical line in the upper-left plot)? In this case, you get the likelihood function $\mathscr{L}(\theta|x=2.5)=\text{f}(x=2.5; \theta)$, represented in the upper-right plot.



Model $f(x;\theta)$
$\mathcal{L}(\theta|x=2.5)=f(x=2.5;\theta)$
θ
$\mathcal{L}$
$\hat{\mathcal{L}}$
Max
$\hat{\theta}$
PDF $f(x;\theta=1.3)$
$\log\mathcal{L}(\theta|x=2.5)$
PDF
$\log\mathcal{L}$
$\log\hat{\mathcal{L}}$
Max
$\hat{\theta}$
x
θ

Figure 9-19. A model's parametric function (top left), and some derived functions: a PDF (lower left), a likelihood function (top right), and a log likelihood function (lower right)

In short, the PDF is a function of x (with θ fixed), while the likelihood function is a function of θ (with x fixed). It is important to understand that the likelihood function is *not* a probability distribution: if you integrate a probability distribution over all possible values of x, you always get 1; but if you integrate the likelihood function over all possible values of θ, the result can be any positive value.

Given a dataset **X**, a common task is to try to estimate the most likely values for the model parameters. To do this, you must find the values that maximize the likelihood function, given **X**. In this example, if you have observed a single instance x=2.5, the *maximum likelihood estimate* (MLE) of θ is $\widehat{\boldsymbol{\theta}}$=1.5. If a prior probability distribution g over θ exists, it is possible to take it into account by maximizing $\mathscr{L}(\theta|x)\mathrm{g}(\theta)$ rather than just maximizing $\mathscr{L}(\theta|x)$. This is called *maximum a-posteriori* (MAP) estimation. Since MAP constrains the parameter values, you can think of it as a regularized version of MLE.

Notice that maximizing the likelihood function is equivalent to maximizing its logarithm (represented in the lower-righthand plot in Figure 9-19). Indeed the logarithm is a strictly increasing function, so if θ maximizes the log likelihood, it also maximizes the likelihood. It turns out that it is generally easier to maximize the log likelihood. For example, if you observed several independent instances $x^{(1)}$ to $x^{(m)}$, you would need to find the value of θ that maximizes the product of the individual likelihood functions. But it is equivalent, and much simpler, to maximize the sum (not the product) of the log likelihood functions, thanks to the magic of the logarithm which converts products into sums: $\log(ab)=\log(a)+\log(b)$.

Once you have estimated $\widehat{\boldsymbol{\theta}}$, the value of θ that maximizes the likelihood function, then you are ready to compute $\widehat{\mathscr{L}} = \mathscr{L}\left(\widehat{\boldsymbol{\theta}}, \mathbf{X}\right)$, which is the value used to compute the AIC and BIC; you can think of it as a measure of how well the model fits the data.

To compute the BIC and AIC, call the `bic()` and `aic()` methods:

```
>>> gm.bic(X)
8189.747000497186
>>> gm.aic(X)
8102.521720382148
```

Figure 9-20 shows the BIC for different numbers of clusters *k*. As you can see, both the BIC and the AIC are lowest when *k*=3, so it is most likely the best choice.

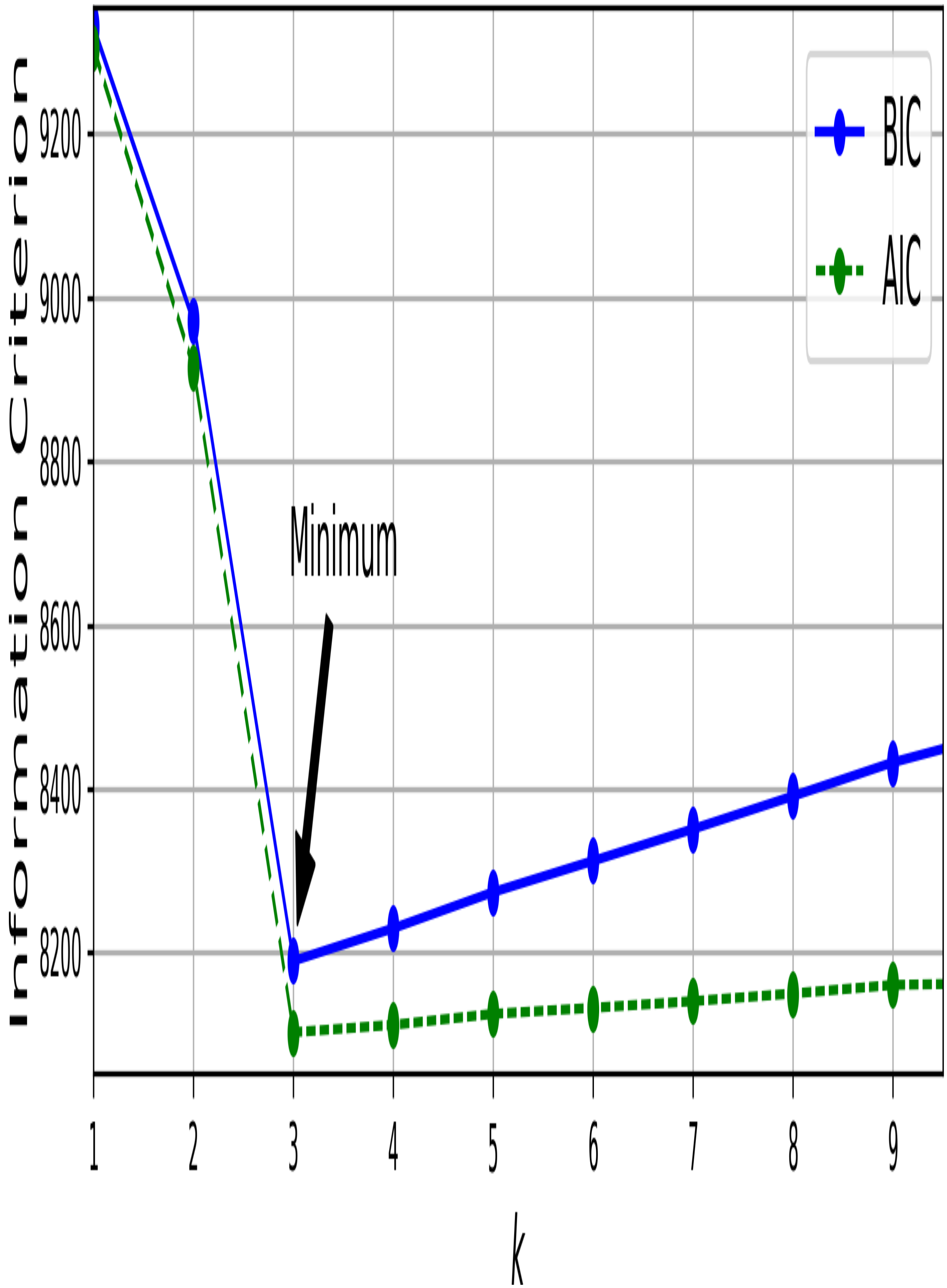


Figure 9-20. AIC and BIC for different numbers of clusters k

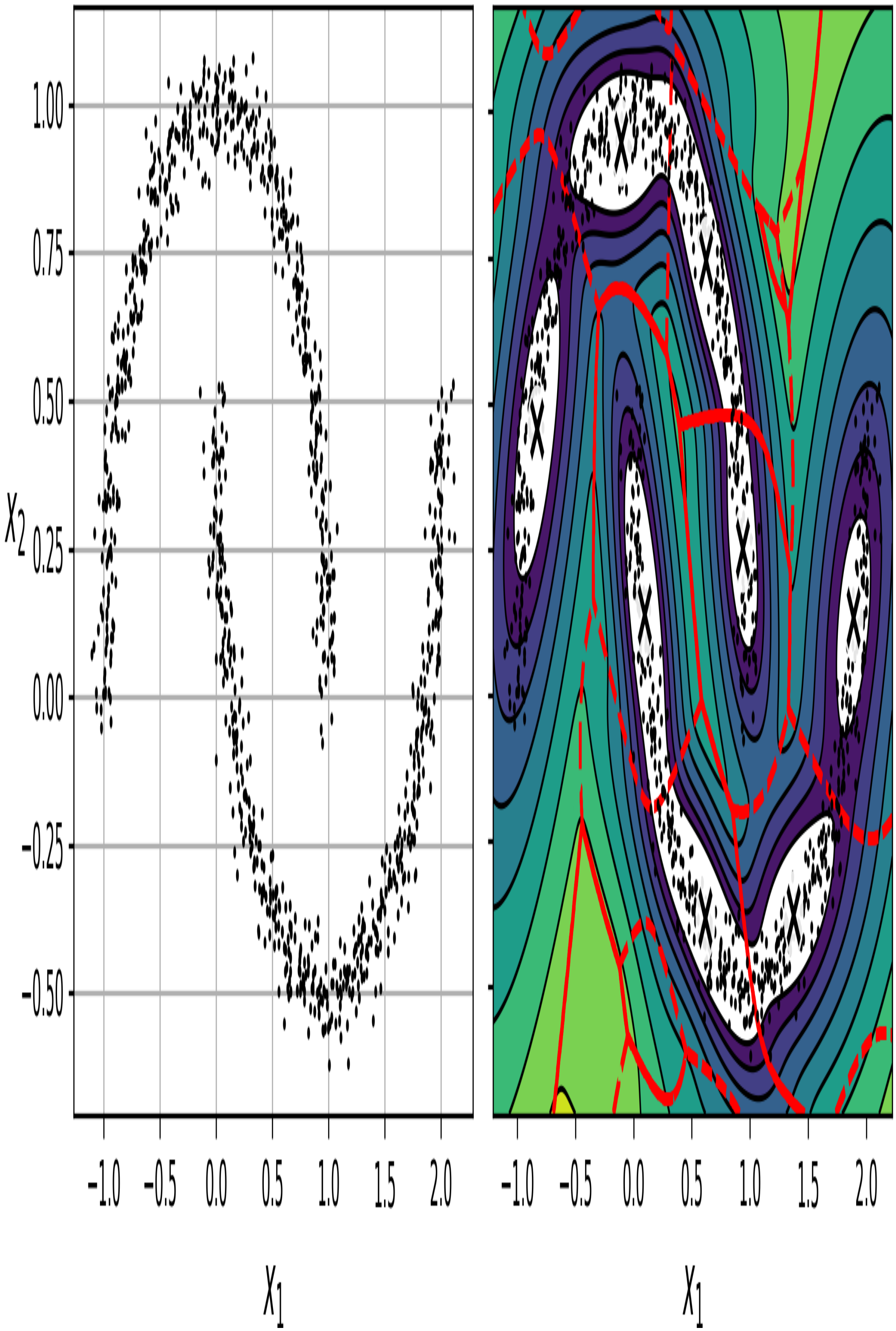
Bayesian Gaussian Mixture Models

Rather than manually searching for the optimal number of clusters, you can use the `BayesianGaussianMixture` class, which is capable of giving weights equal (or close) to zero to unnecessary clusters. Set the number of clusters `n_components` to a value that you have good reason to believe is greater than the optimal number of clusters (this assumes some minimal knowledge about the problem at hand), and the algorithm will eliminate the unnecessary clusters automatically. For example, let's set the number of clusters to 10 and see what happens:

```
>>> from sklearn.mixture import BayesianGaussianMixture
>>> bgm = BayesianGaussianMixture(n_components=10, n_init=10,
random_state=42)
>>> bgm.fit(X)
>>> bgm.weights_.round(2)
array([0.4 , 0.21, 0.4 , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  , 0.
])
```

Perfect: the algorithm automatically detected that only three clusters are needed, and the resulting clusters are almost identical to the ones in Figure 9-16.

A final note about Gaussian mixture models: although they work great on clusters with ellipsoidal shapes, they don't do so well with clusters of very different shapes. For example, let's see what happens if we use a Bayesian Gaussian mixture model to cluster the moons dataset (see Figure 9-21).



1.00
0.75
0.50
0.25
0.00
-0.25
-0.50
X_2
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
X_1
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
X_1

Figure 9-21. Fitting a Gaussian mixture to nonellipsoidal clusters

Oops! The algorithm desperately searched for ellipsoids, so it found eight different clusters instead of two. The density estimation is not too bad, so this model could perhaps be used for anomaly detection, but it failed to identify the two moons. To conclude this chapter, let's take a quick look at a few algorithms capable of dealing with arbitrarily shaped clusters.

Other Algorithms for Anomaly and Novelty Detection

Scikit-Learn implements other algorithms dedicated to anomaly detection or novelty detection:

Fast-MCD (minimum covariance determinant)

Implemented by the `EllipticEnvelope` class, this algorithm is useful for outlier detection, in particular to clean up a dataset. It assumes that the normal instances (inliers) are generated from a single Gaussian distribution (not a mixture). It also assumes that the dataset is contaminated with outliers that were not generated from this Gaussian distribution. When the algorithm estimates the parameters of the Gaussian distribution (i.e., the shape of the elliptic envelope around the inliers), it is careful to ignore the instances that are most likely outliers. This technique gives a better estimation of the elliptic envelope and thus makes the algorithm better at identifying the outliers.

Isolation Forest

This is an efficient algorithm for outlier detection, especially in high-dimensional datasets. The algorithm builds a Random Forest in which each Decision Tree is grown randomly: at each node, it picks a feature randomly, then it picks a random threshold value (between the min and max values) to split the dataset in two. The dataset gradually gets chopped into pieces this way, until all instances end up isolated from the other instances. Anomalies are usually far from other instances, so on average (across all the Decision Trees) they tend to get isolated in fewer steps than normal instances.

Local Outlier Factor (LOF)

This algorithm is also good for outlier detection. It compares the density of instances around a given instance to the density around its neighbors. An anomaly is often more isolated than its *k* nearest neighbors.

One-class SVM

This algorithm is better suited for novelty detection. Recall that a kernelized SVM classifier separates two classes by first (implicitly) mapping all the instances to a high-dimensional space, then separating the two classes using a linear SVM classifier within this high-dimensional space (see Chapter 5). Since we just have one class of instances, the one-class SVM algorithm instead tries to separate the instances in high-dimensional space from the origin. In the original space, this will correspond to finding a small region that encompasses all the instances. If a new instance does not fall within this region, it is an anomaly. There are a few hyperparameters to tweak: the usual ones for a kernelized SVM, plus a margin hyperparameter that corresponds to the probability of a new instance being mistakenly considered as novel when it is in fact normal. It works great, especially with high-dimensional datasets, but like all SVMs it does not scale to large datasets.

PCA and other dimensionality reduction techniques with an `inverse_transform()` method

If you compare the reconstruction error of a normal instance with the reconstruction error of an anomaly, the latter will usually be much larger. This is a simple and often quite efficient anomaly detection approach (see this chapter's exercises for an example).

Exercises

1. How would you define clustering? Can you name a few clustering algorithms?
2. What are some of the main applications of clustering algorithms?
3. Describe two techniques to select the right number of clusters when using K-Means.
4. What is label propagation? Why would you implement it, and how?
5. Can you name two clustering algorithms that can scale to large datasets? And two that look for regions of high density?
6. Can you think of a use case where active learning would be useful? How would you implement it?
7. What is the difference between anomaly detection and novelty detection?
8. What is a Gaussian mixture? What tasks can you use it for?
9. Can you name two techniques to find the right number of clusters when using a Gaussian mixture model?
10. The classic Olivetti faces dataset contains 400 grayscale 64 × 64–pixel images of faces. Each image is flattened to a 1D vector of size 4,096. 40 different people were photographed (10 times each), and the usual task is to train a model that can predict which person is represented in each picture. Load the dataset using the `sklearn.datasets.fetch_olivetti_faces()` function, then split it into a training set, a validation set, and a test set (note that the dataset is already scaled between 0 and 1). Since the dataset is quite small, you probably want to use stratified sampling to ensure that there are the same number of images per person in each set. Next, cluster the images using K-Means, and ensure that you have a good number of clusters (using one of the

techniques discussed in this chapter). Visualize the clusters: do you see similar faces in each cluster?

11. Continuing with the Olivetti faces dataset, train a classifier to predict which person is represented in each picture, and evaluate it on the validation set. Next, use K-Means as a dimensionality reduction tool, and train a classifier on the reduced set. Search for the number of clusters that allows the classifier to get the best performance: what performance can you reach? What if you append the features from the reduced set to the original features (again, searching for the best number of clusters)?

12. Train a Gaussian mixture model on the Olivetti faces dataset. To speed up the algorithm, you should probably reduce the dataset's dimensionality (e.g., use PCA, preserving 99% of the variance). Use the model to generate some new faces (using the `sample()` method), and visualize them (if you used PCA, you will need to use its `inverse_transform()` method). Try to modify some images (e.g., rotate, flip, darken) and see if the model can detect the anomalies (i.e., compare the output of the `score_samples()` method for normal images and for anomalies).

13. Some dimensionality reduction techniques can also be used for anomaly detection. For example, take the Olivetti faces dataset and reduce it with PCA, preserving 99% of the variance. Then compute the reconstruction error for each image. Next, take some of the modified images you built in the previous exercise, and look at their reconstruction error: notice how much larger the reconstruction error is. If you plot a reconstructed image, you will see why: it tries to reconstruct a normal face.

Solutions to these exercises are available at the end of this chapter's notebook, at *https://homl.info/colab3*.

1 Stuart P. Lloyd, “Least Squares Quantization in PCM,” *IEEE Transactions on Information Theory* 28, no. 2 (1982): 129–137.

2 David Arthur and Sergei Vassilvitskii, “k-Means++: The Advantages of Careful Seeding,” *Proceedings of the 18th Annual ACM-SIAM Symposium on Discrete Algorithms* (2007): 1027–1035.

3 Charles Elkan, “Using the Triangle Inequality to Accelerate k-Means,” *Proceedings of the 20th International Conference on Machine Learning* (2003): 147–153.

4 The triangle inequality is AC ≤ AB + BC where A, B and C are three points and AB, AC, and BC are the distances between these points.

5 David Sculley, “Web-Scale K-Means Clustering,” *Proceedings of the 19th International Conference on World Wide Web* (2010): 1177–1178.

6 Phi (ϕ or φ) is the 21st letter of the Greek alphabet.

Part II. Neural Networks and Deep Learning

Chapter 10. Introduction to Artificial Neural Networks with Keras

A NOTE FOR EARLY RELEASE READERS

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.

This will be the 10th chapter of the final book. Notebooks are available on GitHub at *https://github.com/ageron/handson-ml3*. Datasets are available at *https://github.com/ageron/data*.

If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the editoor at ntache@oreilly.com.

Birds inspired us to fly, burdock plants inspired Velcro, and nature has inspired countless more inventions. It seems only logical, then, to look at the brain's architecture for inspiration on how to build an intelligent machine. This is the logic that sparked *artificial neural networks* (ANNs): an ANN is a Machine Learning model inspired by the networks of biological neurons found in our brains. However, although planes were inspired by birds, they don't have to flap their wings. Similarly, ANNs have gradually become quite different from their biological cousins. Some researchers even argue that we should drop the biological analogy altogether (e.g., by saying "units" rather than "neurons"), lest we restrict our creativity to biologically plausible systems.[1]

ANNs are at the very core of Deep Learning. They are versatile, powerful, and scalable, making them ideal to tackle large and highly complex Machine Learning tasks such as classifying billions of images (e.g., Google Images), powering speech recognition services (e.g., Apple's Siri), recommending the best videos to watch to hundreds of millions of users every day (e.g., YouTube), or learning to beat the world champion at the game of Go (DeepMind's AlphaGo).

The first part of this chapter introduces artificial neural networks, starting with a quick tour of the very first ANN architectures and leading up to *Multilayer Perceptrons* (MLPs), which are heavily used today (other architectures will be explored in the next chapters). In the second part, we will look at how to implement neural networks using TensorFlow's Keras API. This is a beautifully designed and simple high-level API for building, training, evaluating, and running neural networks. But don't be fooled by its simplicity: it is expressive and flexible enough to let you build a wide variety of neural network architectures. In fact, it will probably be sufficient for most of your use cases. And should you ever need extra flexibility, you can always write custom Keras components using its lower-level API, or even use TensorFlow directly, as we will see in Chapter 12.

But first, let's go back in time to see how artificial neural networks came to be!

From Biological to Artificial Neurons

Surprisingly, ANNs have been around for quite a while: they were first introduced back in 1943 by the neurophysiologist Warren McCulloch and the mathematician Walter Pitts. In their landmark paper[2] "A Logical Calculus of Ideas Immanent in Nervous Activity," McCulloch and Pitts presented a simplified computational model of how biological neurons might work together in animal brains to perform complex computations using *propositional logic*. This was the first artificial neural network architecture. Since then many other architectures have been invented, as we will see.

The early successes of ANNs led to the widespread belief that we would soon be conversing with truly intelligent machines. When it became clear in the 1960s that this promise would go unfulfilled (at least for quite a while), funding flew elsewhere, and ANNs entered a long winter. In the early 1980s, new architectures were invented and better training techniques were developed, sparking a revival of interest in *connectionism*, the study of neural networks. But progress was slow, and by the 1990s other powerful Machine Learning techniques were invented, such as Support Vector Machines (see Chapter 5). These techniques seemed to offer better results and stronger theoretical foundations than ANNs, so once again the study of neural networks was put on hold.

We are now witnessing yet another wave of interest in ANNs. Will this wave die out like the previous ones did? Well, here are a few good reasons to believe that this time is different and that the renewed interest in ANNs will have a much more profound impact on our lives:

- There is now a huge quantity of data available to train neural networks, and ANNs frequently outperform other ML techniques on very large and complex problems.

- The tremendous increase in computing power since the 1990s now makes it possible to train large neural networks in a reasonable amount of time. This is in part due to Moore's law (the number of components in integrated circuits has doubled about every 2 years over the last 50 years), but also thanks to the gaming industry, which has stimulated the production of powerful GPU cards by the millions. Moreover, cloud platforms have made this power accessible to everyone.

- The training algorithms have been improved. To be fair they are only slightly different from the ones used in the 1990s, but these relatively small tweaks have had a huge positive impact.

- Some theoretical limitations of ANNs have turned out to be benign in practice. For example, many people thought that ANN training algorithms were doomed because they were likely to get stuck in local optima, but it turns out that this is not big problem in practice, especially for larger neural networks: the local optima often perform almost as well as the global optimum.

- ANNs seem to have entered a virtuous circle of funding and progress. Amazing products based on ANNs regularly make the headline news, which pulls more and more attention and funding toward them, resulting in more and more progress and even more amazing products.

Biological Neurons

Before we discuss artificial neurons, let's take a quick look at a biological neuron (represented in Figure 10-1). It is an unusual-looking cell mostly found in animal brains. It's composed of a *cell body* containing the nucleus and most of the cell's complex components, many branching extensions called *dendrites*, plus one very long extension called the *axon*. The axon's length may be just a few times longer than the cell body, or up to tens of thousands of times longer. Near its extremity the axon splits off into many branches called *telodendria*, and at the tip of these branches are minuscule structures called *synaptic terminals* (or simply *synapses*), which are connected to the dendrites or cell bodies of other neurons.[3] Biological neurons produce short electrical impulses called *action potentials* (APs, or just *signals*) which travel along the axons and make the synapses release chemical signals called *neurotransmitters*. When a neuron receives a sufficient amount of these neurotransmitters within a few milliseconds, it fires its own electrical impulses (actually, it depends on the neurotransmitters, as some of them inhibit the neuron from firing).

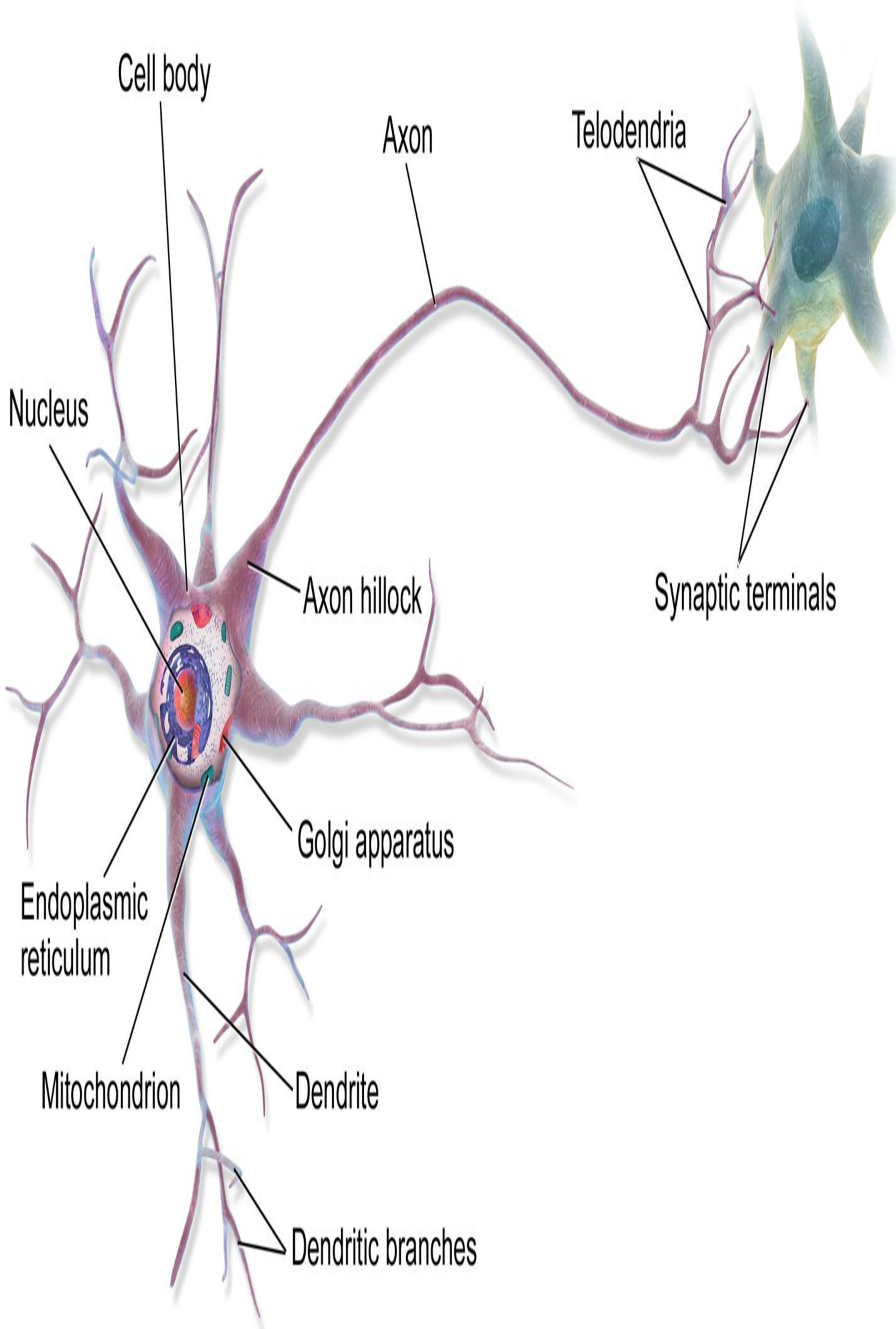

Cell body
Axon
Telodendria
Nucleus
Axon hillock
Synaptic terminals
Golgi apparatus
Endoplasmic reticulum
Mitochondrion
Dendrite
Dendritic branches

Figure 10-1. Biological neuron[4]

Thus, individual biological neurons seem to behave in a rather simple way, but they are organized in a vast network of billions, with each neuron typically connected to thousands of other neurons. Highly complex computations can be performed by a network of fairly simple neurons, much like a complex anthill can emerge from the combined efforts of simple ants. The architecture of biological neural networks (BNNs)[5] is still the subject of active research, but some parts of the brain have been mapped, and it seems that neurons are often organized in consecutive layers, especially in the cerebral cortex (i.e., the outer layer of your brain), as shown in Figure 10-2.

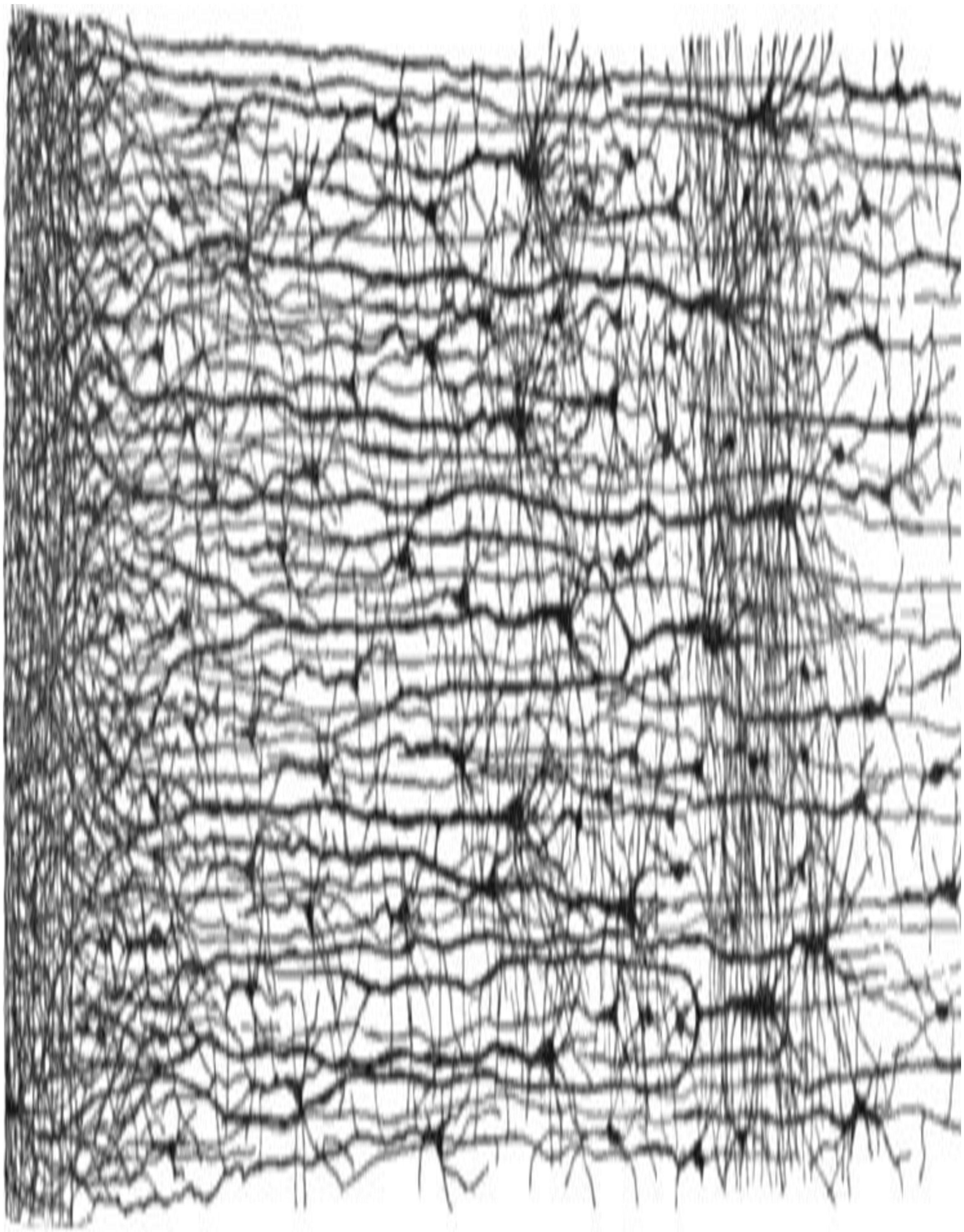


Figure 10-2. Multiple layers in a biological neural network (human cortex)[6]

Logical Computations with Neurons

McCulloch and Pitts proposed a very simple model of the biological neuron, which later became known as an *artificial neuron*: it has one or more binary (on/off) inputs and one binary output. The artificial neuron activates its output when more than a certain number of its inputs are active. In their paper, they showed that even with such a simplified model it is possible to build a network of artificial neurons that computes any logical proposition you want. To see how such a network works, let's build a few ANNs that perform various logical computations (see Figure 10-3), assuming that a neuron is activated when at least two of its input connections are active.

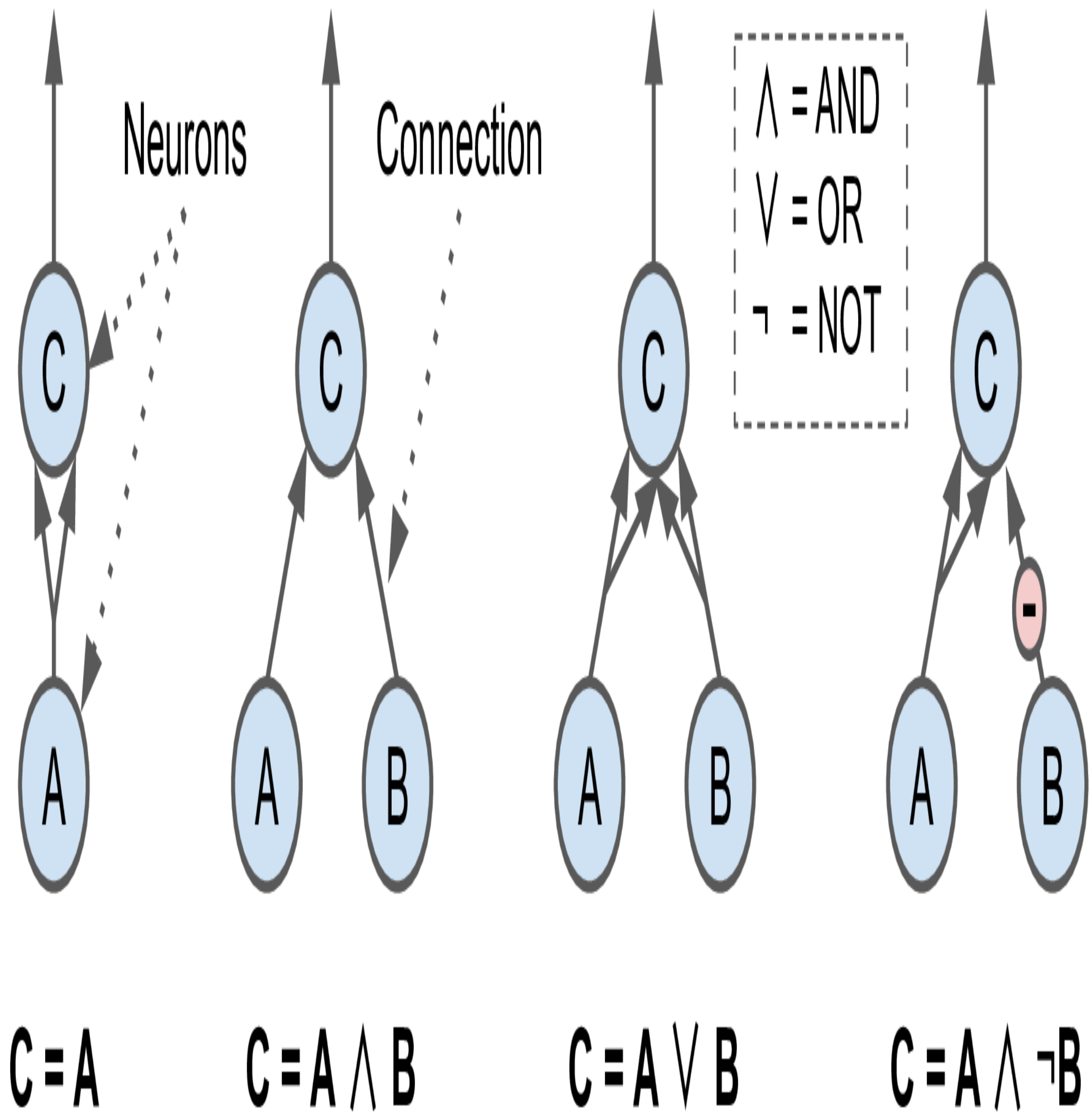


Figure 10-3. ANNs performing simple logical computations

Let's see what these networks do:

- The first network on the left is the identity function: if neuron A is activated, then neuron C gets activated as well (since it receives two input signals from neuron A); but if neuron A is off, then neuron C is off as well.
- The second network performs a logical AND: neuron C is activated only when both neurons A and B are activated (a single input signal is not enough to activate neuron C).

- The third network performs a logical OR: neuron C gets activated if either neuron A or neuron B is activated (or both).
- Finally, if we suppose that an input connection can inhibit the neuron's activity (which is the case with biological neurons), then the fourth network computes a slightly more complex logical proposition: neuron C is activated only if neuron A is active and neuron B is off. If neuron A is active all the time, then you get a logical NOT: neuron C is active when neuron B is off, and vice versa.

You can imagine how these networks can be combined to compute complex logical expressions (see the exercises at the end of the chapter for an example).

The Perceptron

The *Perceptron* is one of the simplest ANN architectures, invented in 1957 by Frank Rosenblatt. It is based on a slightly different artificial neuron (see Figure 10-4) called a *threshold logic unit* (TLU), or sometimes a *linear threshold unit* (LTU). The inputs and output are numbers (instead of binary on/off values), and each input connection is associated with a weight. The TLU first computes a linear function of its inputs: $z = w_1 x_1 + w_2 x_2 + \cdots + w_n x_n + b = \mathbf{w}^\intercal \mathbf{x} + b$. Then it applies a *step function* to the result: $h_{\mathbf{w}}(\mathbf{x}) = \text{step}(z)$. So it's almost like Logistic Regression, except it uses a step function instead of the logistic function (Chapter 4). Just like in Logistic Regression, the model parameters are the input weights $\mathbf{w}$ and the bias term b.

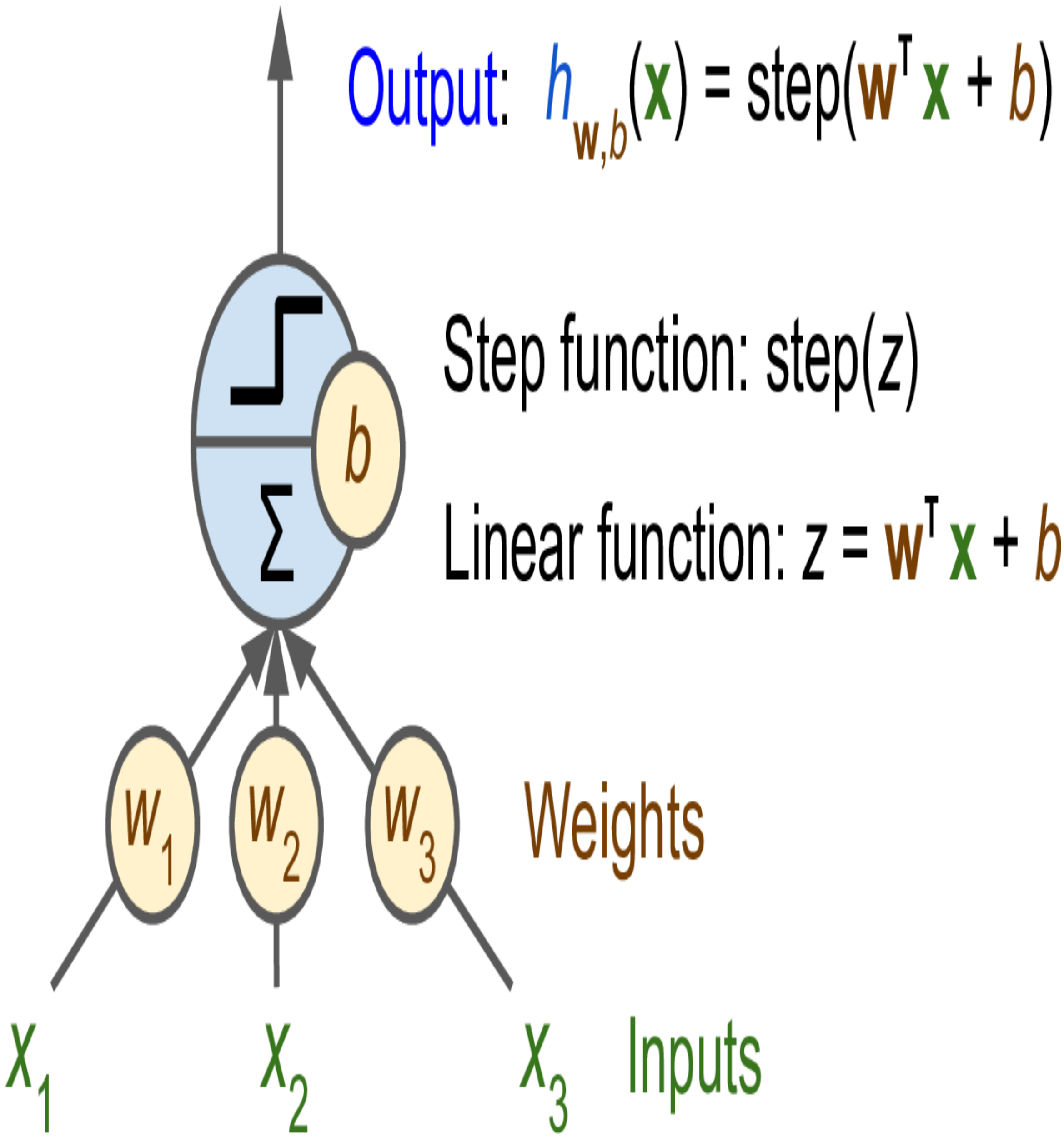


Figure 10-4. Threshold logic unit: an artificial neuron which computes a weighted sum of its inputs $\mathbf{w}^T \mathbf{x}$, plus a bias term b, then applies a step function

The most common step function used in Perceptrons is the *Heaviside step function* (see Equation 10-1). Sometimes the sign function is used instead.

Equation 10-1. Common step functions used in Perceptrons (assuming threshold = 0)

$$\text{heaviside}(z) = \begin{cases} 0 & \text{if } z < 0 \\ 1 & \text{if } z \geq 0 \end{cases} \qquad \text{sgn}(z) = \begin{cases} -1 & \text{if } z < 0 \\ 0 & \text{if } z = 0 \\ +1 & \text{if } z > 0 \end{cases}$$

A single TLU can be used for simple linear binary classification. It computes a linear function of its inputs, and if the result exceeds a threshold, it outputs the positive class. Otherwise it outputs the negative class. This may remind you of Logistic Regression (Chapter 4) or linear SVM classification (Chapter 5). You could, for example, use a single TLU to classify iris flowers based on petal length and width. Training such a TLU would require finding the right values for w_1, w_2 and b (the training algorithm is discussed shortly).

A Perceptron is composed of one or more TLUs organized in a single layer, where every TLU is connected to every input. Such a layer is called a *fully connected layer*, or a *dense layer*. The inputs constitute the *input layer*. And since the layer of TLUs produces the final outputs, it is called the *output layer*. For example, a Perceptron with two inputs and three outputs is represented in Figure 10-5.

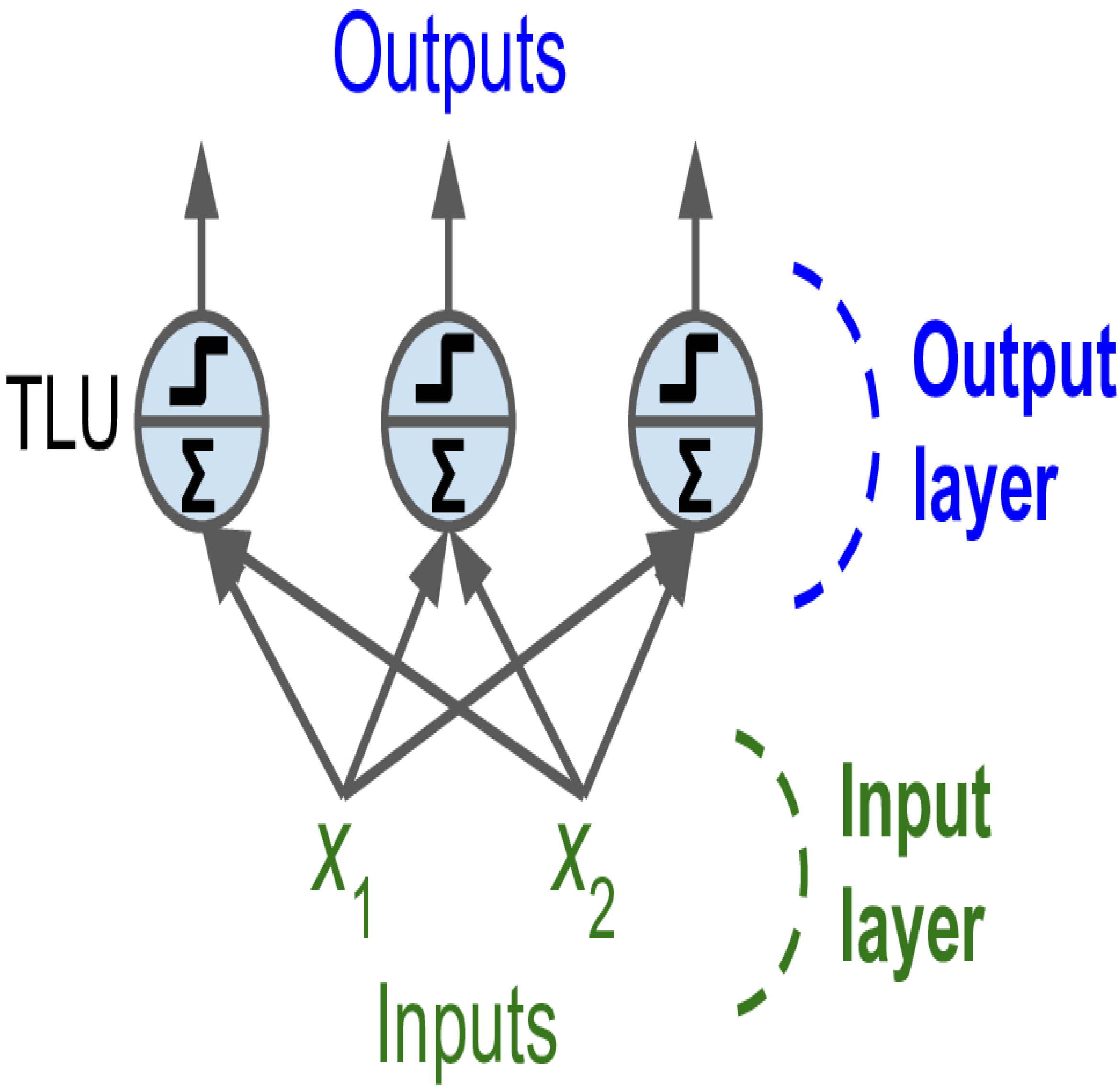


Figure 10-5. Architecture of a Perceptron with two inputs and three output neurons

This Perceptron can classify instances simultaneously into three different binary classes, which makes it a multilabel classifier. It may also be used for multiclass classification.

Thanks to the magic of linear algebra, Equation 10-2 can be used to efficiently compute the outputs of a layer of artificial neurons for several instances at once.

Equation 10-2. Computing the outputs of a fully connected layer

$$h_{\mathbf{W},\mathbf{b}}\left(\mathbf{X}\right) = \phi\left(\mathbf{X}\mathbf{W} + \mathbf{b}\right)$$

In this equation:

- As always, **X** represents the matrix of input features. It has one row per instance and one column per feature.
- The weight matrix **W** contains all the connection weights. It has one row per input and one column per neuron.
- The bias vector **b** contains all the bias terms: one per neuron.
- The function ϕ is called the *activation function*: when the artificial neurons are TLUs, it is a step function (but we will discuss other activation functions shortly).

> **NOTE**
>
> In mathematics, the sum of a matrix and a vector is undefined. However, in Data Science, we allow "broadcasting": adding a vector to a matrix means adding it to every row in the matrix. So **XW** + **b** first multiplies **X** by **W**—which results in a matrix with one row per instance and one column per output—then adds the vector **b** to every row of that matrix, which adds each bias term to the corresponding output, for every instance. Moreover, ϕ is applied itemwise to each item in the resulting matrix.

So, how is a Perceptron trained? The Perceptron training algorithm proposed by Rosenblatt was largely inspired by *Hebb's rule*. In his 1949 book *The Organization of Behavior* (Wiley), Donald Hebb suggested that when a biological neuron triggers another neuron often, the connection between these two neurons grows stronger. Siegrid Löwel later summarized Hebb's idea in the catchy phrase, "Cells that fire together, wire together"; that is, the connection weight between two neurons tends to increase when they fire simultaneously. This rule later became known as Hebb's rule (or *Hebbian learning*). Perceptrons are trained using a variant of this rule that takes into account the error made by the network when it makes a prediction; the Perceptron learning rule reinforces connections that help reduce the error. More specifically, the Perceptron is fed one training instance at a time, and for each instance it makes its predictions. For every output neuron that produced a wrong prediction, it reinforces the connection weights from the inputs that would have contributed to the correct prediction. The rule is shown in Equation 10-3.

Equation 10-3. Perceptron learning rule (weight update)

$$w_{i,j}{}^{(\text{next step})} = w_{i,j} + \eta \left(y_j - \hat{y}_j \right) x_i$$

In this equation:

- $w_{i,j}$ is the connection weight between the i^{th} input and the j^{th} neuron.
- x_i is the i^{th} input value of the current training instance.
- $\hat{y}_j$ is the output of the j^{th} output neuron for the current training instance.
- y_j is the target output of the j^{th} output neuron for the current training instance.
- η is the learning rate (see Chapter 4).

The decision boundary of each output neuron is linear, so Perceptrons are incapable of learning complex patterns (just like Logistic Regression classifiers). However, if the training instances are linearly separable, Rosenblatt demonstrated that this algorithm would converge to a solution.[7] This is called the *Perceptron convergence theorem*.

Scikit-Learn provides a `Perceptron` class which can be used pretty much as you would expect—for example, on the iris dataset (introduced in Chapter 4):

```
import numpy as np
from sklearn.datasets import load_iris
from sklearn.linear_model import Perceptron

iris = load_iris(as_frame=True)
X = iris.data[["petal length (cm)", "petal width (cm)"]].values
y = (iris.target == 0)  # Iris setosa

per_clf = Perceptron(random_state=42)
```

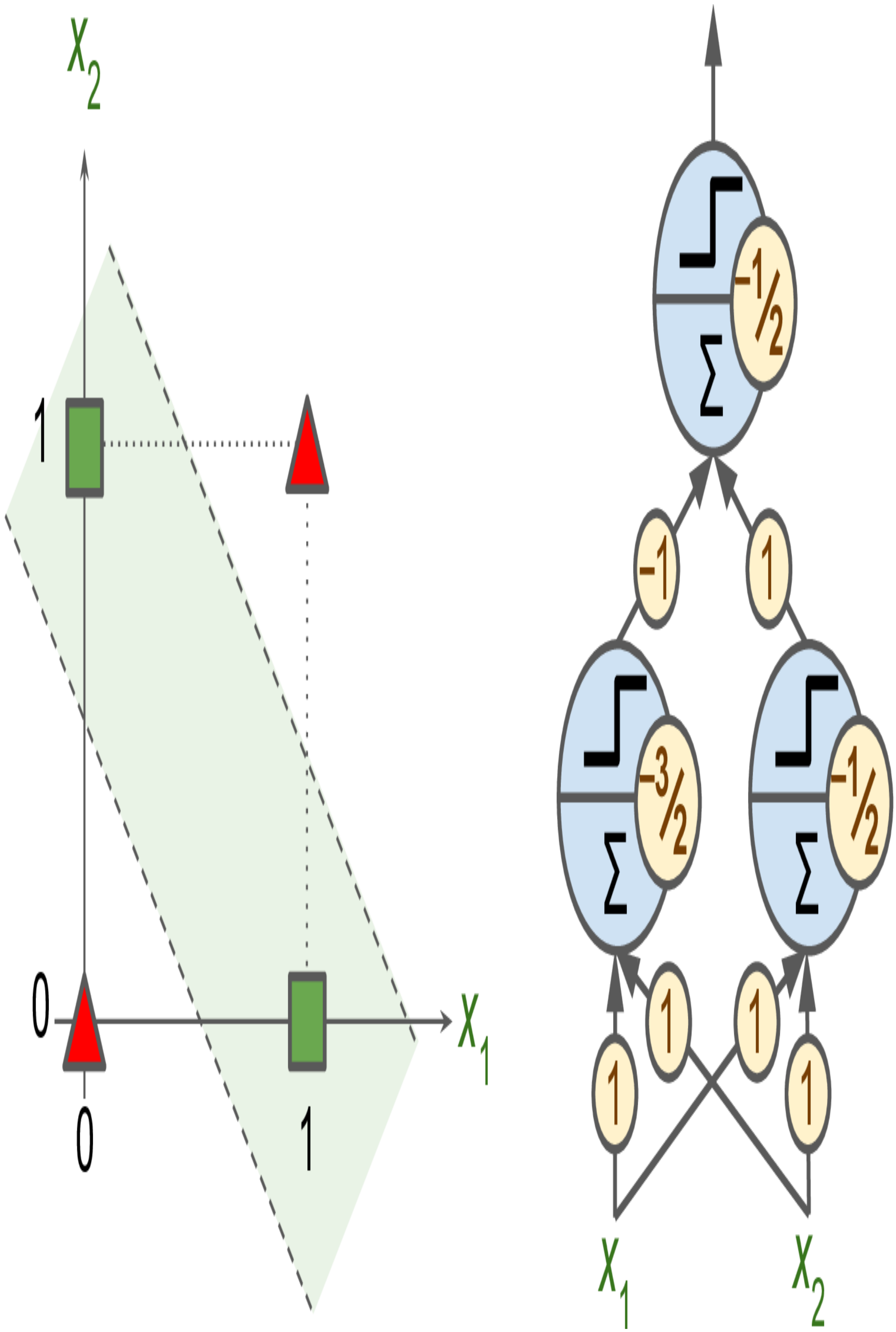
```
per_clf.fit(X, y)

X_new = [[2, 0.5], [3, 1]]
y_pred = per_clf.predict(X_new)  # predicts True and False for
these 2 flowers
```

You may have noticed that the Perceptron learning algorithm strongly resembles Stochastic Gradient Descent (introduced in Chapter 4). In fact, Scikit-Learn's `Perceptron` class is equivalent to using an `SGDClassifier` with the following hyperparameters: `loss="perceptron"`, `learning_rate="constant"`, `eta0=1` (the learning rate), and `penalty=None` (no regularization).

> **NOTE**
>
> Contrary to Logistic Regression classifiers, Perceptrons do not output a class probability. This is one reason to prefer Logistic Regression over Perceptrons. Moreover, Perceptrons do not use any regularization by default, and training stops as soon as there are no more prediction errors on the training set, so the model typically does not generalize as well as Logistic Regression or a linear SVM classifier. However, Perceptrons may train a bit faster.

In their 1969 monograph *Perceptrons*, Marvin Minsky and Seymour Papert highlighted a number of serious weaknesses of Perceptrons—in particular, the fact that they are incapable of solving some trivial problems (e.g., the *Exclusive OR* (XOR) classification problem; see the left side of Figure 10-6). This is true of any other linear classification model (such as Logistic Regression classifiers), but researchers had expected much more from Perceptrons, and some were so disappointed that they dropped neural networks altogether in favor of higher-level problems such as logic, problem solving, and search.

It turns out that some of the limitations of Perceptrons can be eliminated by stacking multiple Perceptrons. The resulting ANN is called a *Multilayer Perceptron* (MLP). An MLP can solve the XOR problem, as you can verify by computing the output of the MLP represented on the right side of Figure 10-6: with inputs (0, 0) or (1, 1), the network outputs 0, and with inputs (0, 1) or (1, 0) it outputs 1. Try verifying that this network indeed solves the XOR problem![8]



x2
1
0
x1
0
1
−1
1
−1/2
−3/2
1
1
1
1
x1
x2

Figure 10-6. XOR classification problem and an MLP that solves it

The Multilayer Perceptron and Backpropagation

An MLP is composed of one input layer, one or more layers of TLUs, called *hidden layers*, and one final layer of TLUs called the *output layer* (see Figure 10-7). The layers close to the input layer are usually called the *lower layers*, and the ones close to the outputs are usually called the *upper layers*.

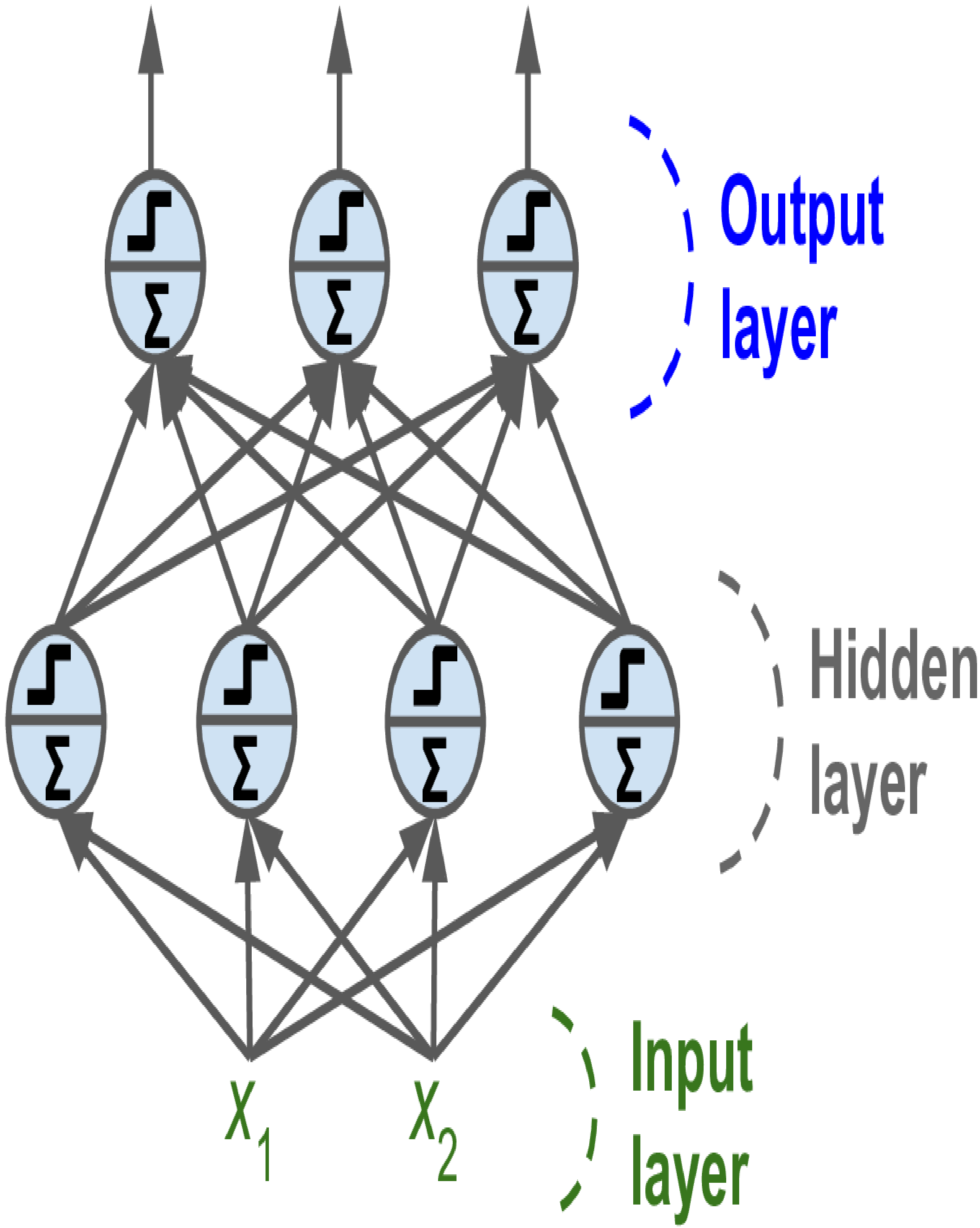


Figure 10-7. Architecture of a Multilayer Perceptron with two inputs, one hidden layer of four neurons, and three output neurons

NOTE

The signal flows only in one direction (from the inputs to the outputs), so this architecture is an example of a *feedforward neural network* (FNN).

When an ANN contains a deep stack of hidden layers,[9] it is called a *deep neural network* (DNN). The field of Deep Learning studies DNNs, and more generally it is interested in models containing deep stacks of computations. Even so, many people talk about Deep Learning whenever neural networks are involved (even shallow ones).

For many years researchers struggled to find a way to train MLPs, without success. In the early 1960s, several researchers discussed the possibility to use Gradient Descent to train neural networks, but as we saw in Chapter 4, Gradient Descent requires computing the gradients of the model's error with regards to the model parameters: it wasn't clear at the time how to do this efficiently with such a complex model containing so many parameters, especially with the computers they had back then.

Then in 1970, a researcher named Seppo Linnainmaa introduced, in his master thesis, a technique to compute all the gradients automatically and efficiently. This algorithm is now called *reverse-mode automatic differentiation* (or *reverse-mode autodiff* for short). In just two passes through the network (one forward, one backward), it is able to compute the gradients of the neural network's error with regard to every single model parameter. In other words, it can find out how each connection weight and each bias should be tweaked in order to reduce the neural network's error. These gradients can then be used to perform a Gradient Descent step. If you repeat this process of computing the gradients automatically and taking a Gradient Descent step, the neural network's error will gradually drop, until it eventually reaches a minimum. This combination of reverse-mode autodiff and Gradient Descent is now called *backpropagation* (or *backprop* for short).

NOTE

There are various autodiff techniques, with different pros and cons. *Reverse-mode autodiff* is well suited when the function to differentiate has many variables (e.g., connection weights and biases) and few outputs (e.g., one loss). If you want to learn more about autodiff, check out Appendix B.

Backpropagation can actually be applied to all sorts of computational graphs, not just neural networks: indeed, Linnainmaa's master thesis was not about neural nets, it was more general. It took several more years before backprop started to be used to train neural networks, but it still wasn't mainstream. Then David Rumelhart reinvented backpropagation (as did several other researchers in other fields), and he published a groundbreaking paper[10] in 1986, along with Geoffrey Hinton and Ronald Williams, analyzing how backpropagation allowed neural networks to learn useful internal representations. Their results were so impressive that backpropagation was quickly popularized in the field. Today, it is by far the most popular training technique for neural networks.

So let's run through backpropagation again in a bit more detail:

- It handles one mini-batch at a time (for example, containing 32 instances each), and it goes through the full training set multiple times. Each pass is called an *epoch*.
- Each mini-batch enters the network through the input layer. The algorithm then computes the output of all the neurons in the first hidden layer, for every instance in the mini-batch. The result is passed on to the next layer, its output is computed and passed to the next layer, and so on until we get the output of the last layer, the output layer. This is the *forward pass*: it is exactly like making predictions, except all intermediate results are preserved since they are needed for the backward pass.
- Next, the algorithm measures the network's output error (i.e., it uses a loss function that compares the desired output and the actual

output of the network, and returns some measure of the error).

- Then it computes how much each output bias and each connection to the output layer contributed to the error. This is done analytically by applying the *chain rule* (perhaps the most fundamental rule in calculus), which makes this step fast and precise.

- The algorithm then measures how much of these error contributions came from each connection in the layer below, again using the chain rule, working backward until the algorithm reaches the input layer. As explained earlier, this reverse pass efficiently measures the error gradient across all the connection weights and biases in the network by propagating the error gradient backward through the network (hence the name of the algorithm).

- Finally, the algorithm performs a Gradient Descent step to tweak all the connection weights in the network, using the error gradients it just computed.

In short, backpropagation makes predictions for a mini-batch (forward pass), measures the error, then goes through each layer in reverse to measure the error contribution from each parameter (reverse pass), and finally tweaks the connection weights and biases to reduce the error (Gradient Descent step).

WARNING

It is important to initialize all the hidden layers' connection weights randomly, or else training will fail. For example, if you initialize all weights and biases to zero, then all neurons in a given layer will be perfectly identical, and thus backpropagation will affect them in exactly the same way, so they will remain identical. In other words, despite having hundreds of neurons per layer, your model will act as if it had only one neuron per layer: it won't be too smart. If instead you randomly initialize the weights, you *break the symmetry* and allow backpropagation to train a diverse team of neurons.

In order for backprop to work properly, Rumelhart and his colleagues made a key change to the MLP's architecture: they replaced the step function with the logistic function, $\sigma(z) = 1 / (1 + \exp(-z))$, also called the *sigmoid* function. This was essential because the step function contains only flat segments, so there is no gradient to work with (Gradient Descent cannot move on a flat surface), while the sigmoid function has a well-defined nonzero derivative everywhere, allowing Gradient Descent to make some progress at every step. In fact, the backpropagation algorithm works well with many other activation functions, not just the sigmoid function. Here are two other popular choices:

The hyperbolic tangent function: $\tanh(z) = 2\sigma(2z) - 1$

Just like the sigmoid function, this activation function is *S*-shaped, continuous, and differentiable, but its output value ranges from –1 to 1 (instead of 0 to 1 in the case of the sigmoid function). That range tends to make each layer's output more or less centered around 0 at the beginning of training, which often helps speed up convergence.

The Rectified Linear Unit function: $\text{ReLU}(z) = \max(0, z)$

The ReLU function is continuous but unfortunately not differentiable at $z = 0$ (the slope changes abruptly, which can make Gradient Descent bounce around), and its derivative is 0 for $z < 0$. In practice, however, it works very well and has the advantage of being fast to compute, so it has become the default.[11] Importantly, the fact that it does not have a maximum output value helps reduce some issues during Gradient Descent (we will come back to this in Chapter 11).

These popular activation functions and their derivatives are represented in Figure 10-8. But wait! Why do we need activation functions in the first place? Well, if you chain several linear transformations, all you get is a linear transformation. For example, if $f(x) = 2x + 3$ and $g(x) = 5x - 1$, then chaining these two linear functions gives you another linear function: $f(g(x)) = 2(5x - 1) + 3 = 10x + 1$. So if you don't have some nonlinearity between layers, then even a deep stack of layers is equivalent to a single layer, and you can’t solve very complex problems with that. Conversely, a large enough DNN with nonlinear activations can theoretically approximate any continuous function.

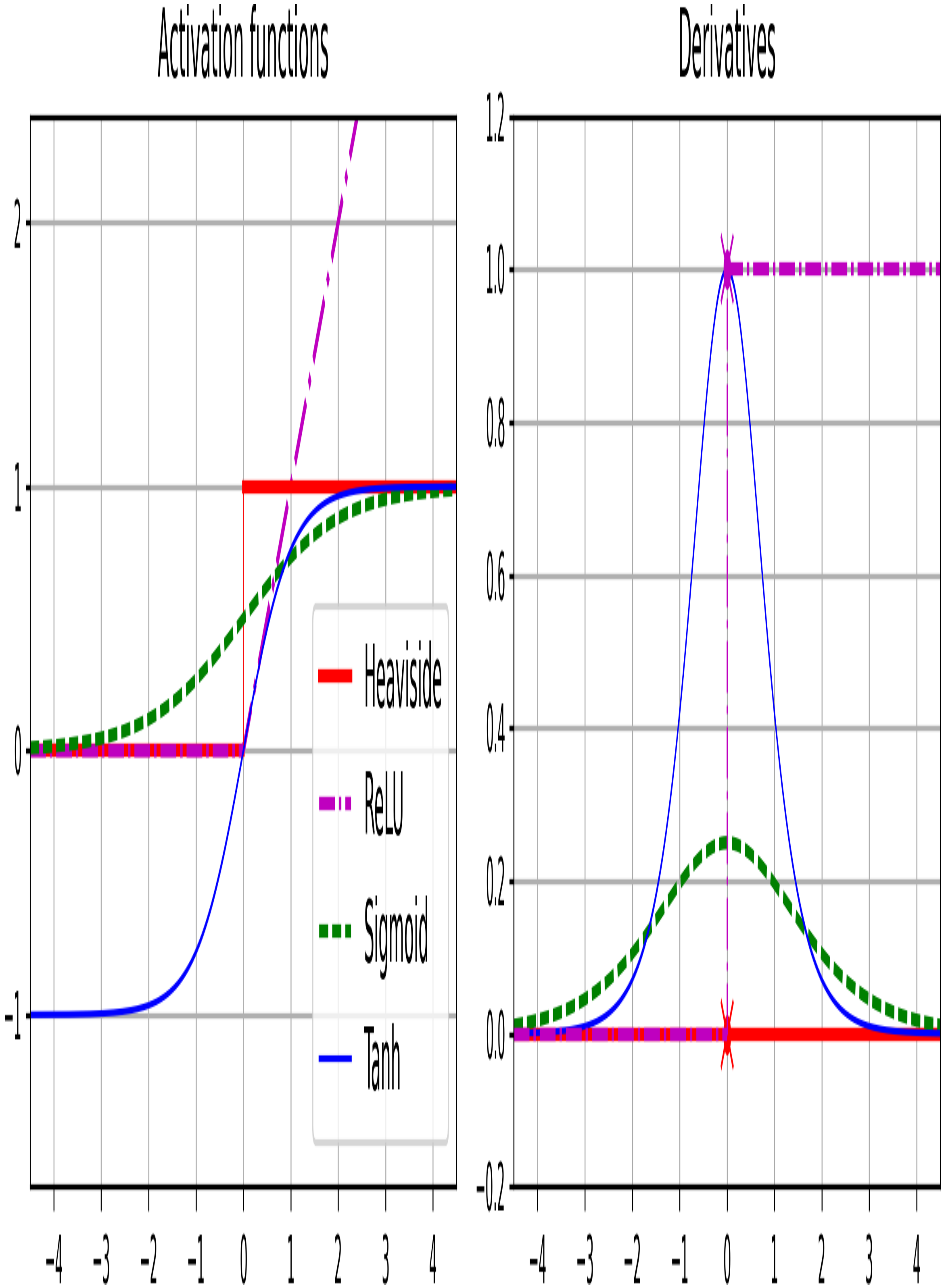


Figure 10-8. Activation functions (left) and their derivatives (right)

OK! You know where neural nets came from, what their architecture is, and how to compute their outputs. You've also learned about the backpropagation algorithm. But what exactly can you do with neural nets?

Regression MLPs

First, MLPs can be used for regression tasks. If you want to predict a single value (e.g., the price of a house, given many of its features), then you just need a single output neuron: its output is the predicted value. For multivariate regression (i.e., to predict multiple values at once), you need one output neuron per output dimension. For example, to locate the center of an object in an image, you need to predict 2D coordinates, so you need two output neurons. If you also want to place a bounding box around the object, then you need two more numbers: the width and the height of the object. So, you end up with four output neurons.

Scikit-Learn includes an `MLPRegressor` class, so let's use it to build an MLP with three hidden layers composed of 50 neurons each, and train it on the California housing dataset. For simplicity, we will use Scikit-Learn's `fetch_california_housing()` function to load the data. This dataset is simpler than the one we used in Chapter 2, since it contains only numerical features (there is no `ocean_proximity` feature), and there are no missing values. The following code starts by fetching and splitting the dataset, then it creates a pipeline to standardize the input features before sending them to the `MLPRegressor`. This is very important for neural networks because they are trained using Gradient Descent, and as we saw in Chapter 4, Gradient Descent does not converge very well when the features have very different scales. Finally, the code trains the model and evaluates its validation error. The model uses the ReLU activation function in the hidden layers, and it uses a variant of Gradient Descent called *Adam* (see Chapter 11) to minimize the mean squared error, with a little bit of ℓ_2 regularization (which you can control via the `alpha` hyperparameter).

```
from sklearn.datasets import fetch_california_housing
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import train_test_split
```

```
from sklearn.neural_network import MLPRegressor
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler

housing = fetch_california_housing()
X_train_full, X_test, y_train_full, y_test = train_test_split(
    housing.data, housing.target, random_state=42)
X_train, X_valid, y_train, y_valid = train_test_split(
    X_train_full, y_train_full, random_state=42)

mlp_reg = MLPRegressor(hidden_layer_sizes=[50, 50, 50],
random_state=42)
pipeline = make_pipeline(StandardScaler(), mlp_reg)
pipeline.fit(X_train, y_train)
y_pred = pipeline.predict(X_valid)
rmse = mean_squared_error(y_valid, y_pred, squared=False)  #
about 0.505
```

We get a validation RMSE of about 0.505, which is comparable to what you would get with a Random Forest classifier. Not too bad for a first try!

Note that this MLP does not use any activation function for the output layer, so it's free to output any value it wants. This is generally fine, but if you want to guarantee that the output will always be positive, then you should use the ReLU activation function in the output layer, or the *softplus* activation function, which is a smooth variant of ReLU: softplus(z) = log(1 + exp(z)). Softplus is close to 0 when z is negative, and close to z when z is positive. Finally, if you want to guarantee that the predictions will always fall within a given range of values, then you should use the sigmoid function or the hyperbolic tangent, and scale the targets to the appropriate range: 0 to 1 for sigmoid and –1 to 1 for tanh. Sadly, the `MLPRegressor` class does not support activation functions in the output layer.

WARNING

Building and training a standard MLP with Scikit-Learn in just a few lines of code is very convenient, but the neural net features are limited. This is why we will switch to Keras in the second part of this chapter.

The `MLPRegressor` class uses the mean squared error, which is usually what you want for regression, but if you have a lot of outliers in the training set, you may prefer to use the mean absolute error instead. Alternatively, you may want to use the Huber loss, which is a combination of both. It is quadratic when the error is smaller than a threshold δ (typically 1) but linear when the error is larger than δ. The linear part makes it less sensitive to outliers than the mean squared error, and the quadratic part allows it to converge faster and be more precise than the mean absolute error. However, `MLPRegressor` only supports the MSE.

Table 10-1 summarizes the typical architecture of a regression MLP.

Table 10-1. Typical regression MLP arc

h
i
t
e
c
t
u
r
e

Hyperparameter	Typical value
# hidden layers	Depends on the problem, but typically 1 to 5
# neurons per hidden layer	Depends on the problem, but typically 10 to 100
# output neurons	1 per prediction dimension
Hidden activation	ReLU
Output activation	None, or ReLU/softplus (if positive outputs) or sigmoid/tanh (if bounded outputs)
Loss function	MSE, or Huber if outliers

Classification MLPs

MLPs can also be used for classification tasks. For a binary classification problem, you just need a single output neuron using the sigmoid activation function: the output will be a number between 0 and 1, which you can interpret as the estimated probability of the positive class. The estimated probability of the negative class is equal to one minus that number.

MLPs can also easily handle multilabel binary classification tasks (see Chapter 3). For example, you could have an email classification system that predicts whether each incoming email is ham or spam, and simultaneously predicts whether it is an urgent or nonurgent email. In this case, you would need two output neurons, both using the sigmoid activation function: the first would output the probability that the email is spam, and the second would output the probability that it is urgent. More generally, you would dedicate one output neuron for each positive class. Note that the output probabilities do not necessarily add up to 1. This lets the model output any combination of labels: you can have nonurgent ham, urgent ham, nonurgent spam, and perhaps even urgent spam (although that would probably be an error).

If each instance can belong only to a single class, out of three or more possible classes (e.g., classes 0 through 9 for digit image classification), then you need to have one output neuron per class, and you should use the softmax activation function for the whole output layer (see Figure 10-9). The softmax function (introduced in Chapter 4) will ensure that all the estimated probabilities are between 0 and 1, and that they add up to 1 since the classes are exclusive. This is called multiclass classification.

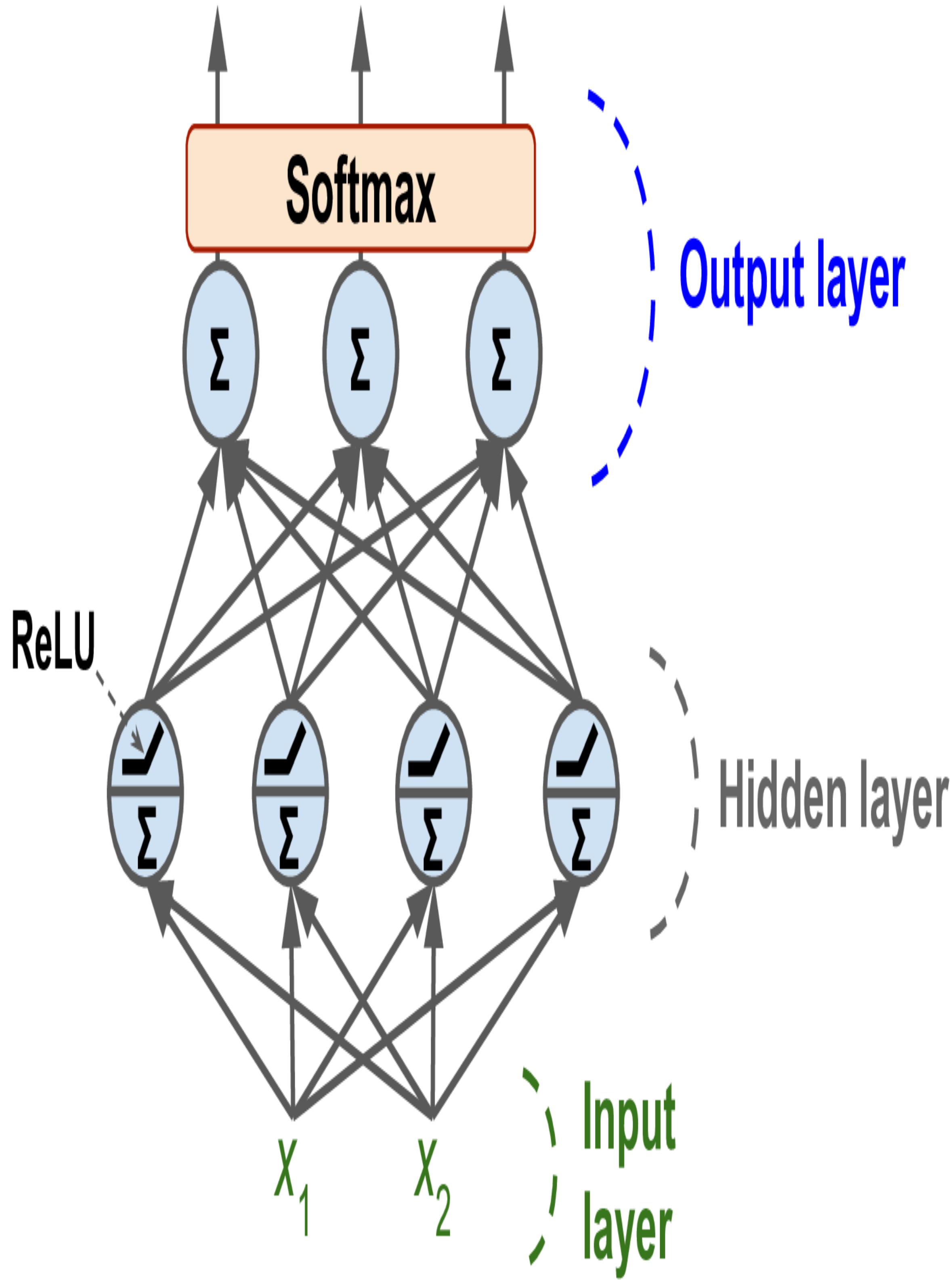


Figure 10-9. A modern MLP (including ReLU and softmax) for classification

Regarding the loss function, since we are predicting probability distributions, the cross-entropy loss (or *x-entropy* or log loss for short, see Chapter 4) is generally a good choice.

Scikit-Learn has an `MLPClassifier` class in the `sklearn.neural_network` package. It is almost identical to the `MLPRegressor` class, except that it minimizes the cross-entropy rather than the MSE. Give it a try now, for example on the Iris dataset. It's a almost a linear task, so a single layer with 5 to 10 neurons should suffice (and make sure to scale the features).

Table 10-2 summarizes the typical architecture of a classification MLP.

Table 10-2. Typical classification MLP *architecture*

Hyperparameter	Binary classification	Multilabel binary classification	Multiclass classification
hidden layers	Same as regression	Same as regression	Same as regression
# output neurons	1	1 per binary label	1 per class
Output layer activation	Sigmoid	Sigmoid	Softmax
Loss function	x-entropy	x-entropy	x-entropy

> **TIP**
>
> Before we go on, I recommend you go through exercise 1 at the end of this chapter. You will play with various neural network architectures and visualize their outputs using the *TensorFlow Playground*. This will be very useful to better understand MLPs, including the effects of all the hyperparameters (number of layers and neurons, activation functions, and more).

Now you have all the concepts you need to start implementing MLPs with Keras!

Implementing MLPs with Keras

Keras is TensorFlow's high-level Deep Learning API: it allows you to build, train, evaluate, and execute all sorts of neural networks. The original Keras library was developed by François Chollet as part of a research project[12] and was released as a standalone open source project in March 2015. It quickly gained popularity, owing to its ease of use, flexibility, and beautiful design.

> **NOTE**
>
> Keras used to support multiple backends, including TensorFlow, PlaidML, Theano and Microsoft Cognitive Toolkit (CNTK) (the last two are sadly deprecated), but since version 2.4, Keras is TensorFlow-only. Conversely, TensorFlow used to include multiple high-level APIs, but Keras was officially chosen as its preferred high-level API when TensorFlow 2 came out. Installing TensorFlow will automatically install Keras as well, and Keras will not work without TensorFlow installed. In short, Keras and TensorFlow fell in love and got married. François Chollet joined Google where he continues to lead the Keras project.

The most popular Deep Learning library, after Keras and TensorFlow, is Facebook's PyTorch library. The good news is that its API is quite similar to Keras's, in part because both APIs were inspired by Scikit-Learn and Chainer. So once you know Keras, it is not difficult to switch to PyTorch, if you ever want to. PyTorch's popularity grew exponentially in 2018, largely thanks to its simplicity and excellent documentation, which were not TensorFlow 1.x's main strengths back then. However, TensorFlow 2 is just as simple as PyTorch, in part because it has adopted Keras as its official high-level API, but also because the developers have greatly simplified and cleaned up the rest of the API. The documentation has also been completely reorganized, and it is much easier to find what you need now. Similarly, PyTorch's main weaknesses (e.g., limited portability and no computation graph analysis) have been largely addressed in PyTorch 1.0. Healthy competition seems beneficial to everyone.

All right, now let's use Keras! We will start by building an MLP for image classification using Keras.

> **NOTE**
>
> Colab Runtimes come with recent versions of TensorFlow and Keras preinstalled. However, if you want to install them on your own machine, please see the installation instructions at *https://homl.info/install*.

Building an Image Classifier Using the Sequential API

First, we need to load a dataset. We will use Fashion MNIST, which is a drop-in replacement of MNIST (introduced in Chapter 3). It has the exact same format as MNIST (70,000 grayscale images of 28 × 28 pixels each, with 10 classes), but the images represent fashion items rather than handwritten digits, so each class is more diverse, and the problem turns out to be significantly more challenging than MNIST. For example, a simple linear model reaches about 92% accuracy on MNIST, but only about 83% on Fashion MNIST.

Using Keras to load the dataset

Keras provides some utility functions to fetch and load common datasets, including MNIST, Fashion MNIST, and a few more. Let's load Fashion MNIST. It's already shuffled and split into a training set (60,000 images) and a test set (10,000 images), but let's hold out the last 5,000 images from the training set for validation:

```
import tensorflow as tf

fashion_mnist = tf.keras.datasets.fashion_mnist.load_data()
(X_train_full, y_train_full), (X_test, y_test) = fashion_mnist
X_train, y_train = X_train_full[:-5000], y_train_full[:-5000]
X_valid, y_valid = X_train_full[-5000:], y_train_full[-5000:]
```

> **TIP**
>
> TensorFlow is usually imported as `tf`, and the Keras API is available via `tf.keras`.

When loading MNIST or Fashion MNIST using Keras rather than Scikit-Learn, one important difference is that every image is represented as a 28 × 28 array rather than a 1D array of size 784. Moreover, the pixel intensities are represented as integers (from 0 to 255) rather than floats (from 0.0 to 255.0). Let's take a look at the shape and data type of the training set:

```
>>> X_train.shape
(55000, 28, 28)
>>> X_train.dtype
dtype('uint8')
```

For simplicity, we'll scale the pixel intensities down to the 0–1 range by dividing them by 255.0 (this also converts them to floats):

```
X_train, X_valid, X_test = X_train / 255., X_valid / 255., X_test
/ 255.
```

With MNIST, when the label is equal to 5, it means that the image represents the handwritten digit 5. Easy. For Fashion MNIST, however, we need the list of class names to know what we are dealing with:

```
class_names = ["T-shirt/top", "Trouser", "Pullover", "Dress",
"Coat",
               "Sandal", "Shirt", "Sneaker", "Bag", "Ankle boot"]
```

For example, the first image in the training set represents an ankle boot:

```
>>> class_names[y_train[0]]
'Ankle boot'
```

Figure 10-10 shows some samples from the Fashion MNIST dataset.

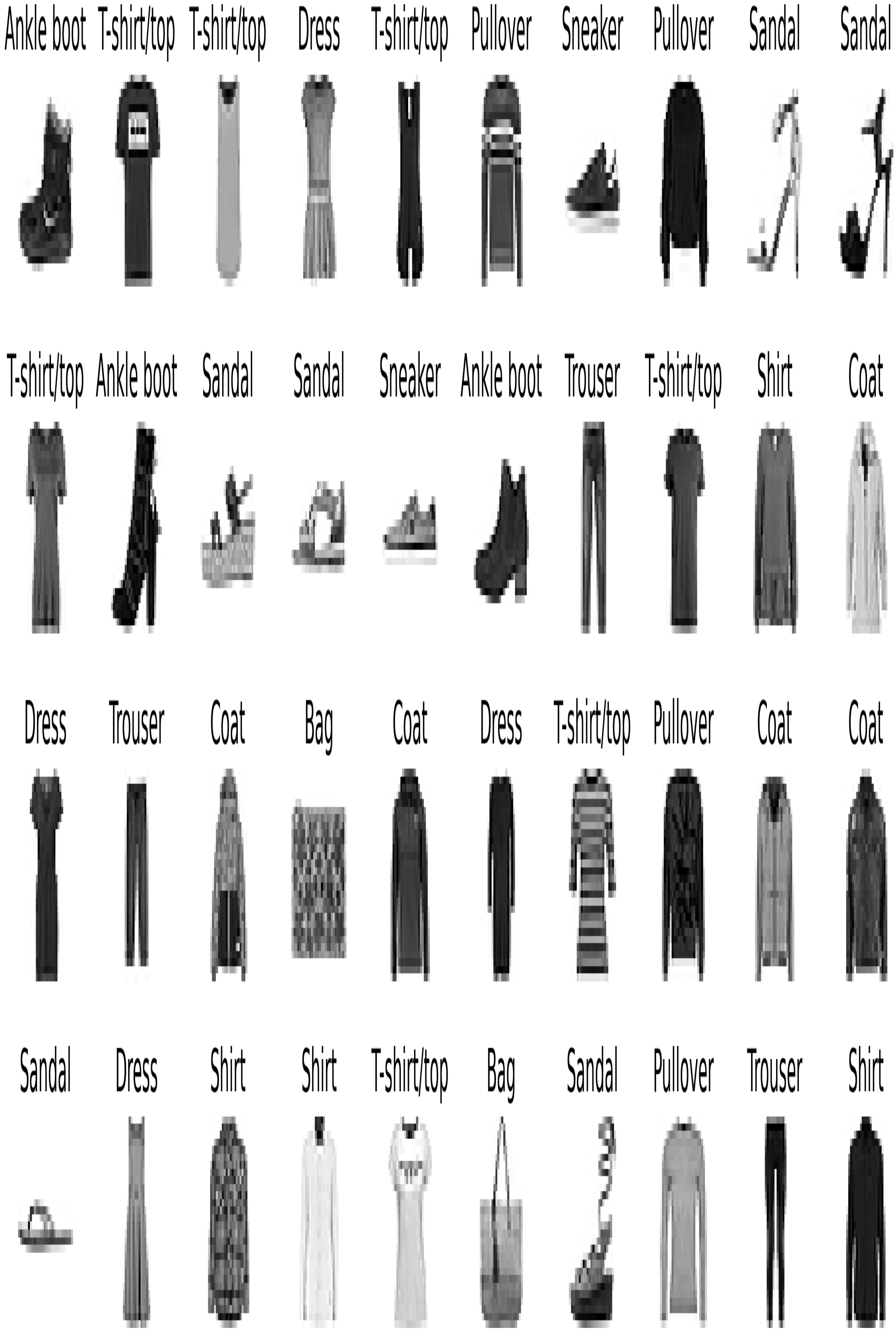

Ankle boot
T-shirt/top
T-shirt/top
Dress
T-shirt/top
Pullover
Sneaker
Pullover
Sandal
Sandal
T-shirt/top
Ankle boot
Sandal
Sandal
Sneaker
Ankle boot
Trouser
T-shirt/top
Shirt
Coat
Dress
Trouser
Coat
Bag
Coat
Dress
T-shirt/top
Pullover
Coat
Coat
Sandal
Dress
Shirt
Shirt
T-shirt/top
Bag
Sandal
Pullover
Trouser
Shirt

Figure 10-10. Samples from Fashion MNIST

Creating the model using the Sequential API

Now let's build the neural network! Here is a classification MLP with two hidden layers:

```
tf.random.set_seed(42)
model = tf.keras.Sequential()
model.add(tf.keras.layers.InputLayer(input_shape=[28, 28]))
model.add(tf.keras.layers.Flatten())
model.add(tf.keras.layers.Dense(300, activation="relu"))
model.add(tf.keras.layers.Dense(100, activation="relu"))
model.add(tf.keras.layers.Dense(10, activation="softmax"))
```

Let's go through this code line by line:

- We first set TensorFlow's random seed to make the results reproducible: the random weights of the hidden layers and the output layer will be the same every time you run the notebook.
- The next line creates a `Sequential` model. This is the simplest kind of Keras model for neural networks that are just composed of a single stack of layers connected sequentially. This is called the Sequential API.
- Next, we build the first layer and add it to the model: it is an `InputLayer`. We specify the `input_shape`, which doesn't include the batch size, only the shape of the instances. Keras needs to know the shape of the inputs so it can determine the shape of the connection weight matrix of the first hidden layer.
- Then we add a `Flatten` layer whose role is to convert each input image into a 1D array: for example, if it receives a batch of shape [32, 28, 28], it will reshape it to [32, 784]. In other words, if it receives input data `X`, it computes `X.reshape(-1, 784)`. This layer does not have any parameters; it is just there to do some simple preprocessing.

- Next we add a `Dense` hidden layer with 300 neurons. It will use the ReLU activation function. Each `Dense` layer manages its own weight matrix, containing all the connection weights between the neurons and their inputs. It also manages a vector of bias terms (one per neuron). When it receives some input data, it computes Equation 10-2.

- Then we add a second `Dense` hidden layer with 100 neurons, also using the ReLU activation function.

- Finally, we add a `Dense` output layer with 10 neurons (one per class), using the softmax activation function because the classes are exclusive.

> **TIP**
>
> Specifying `activation="relu"` is equivalent to specifying `activation=tf.keras.activations.relu`. Other activation functions are available in the `tf.keras.activations` package, we will use many of them in this book. See *https://keras.io/api/layers/activations/* for the full list. We will also define our own custom activation functions in Chapter 12.

Instead of adding the layers one by one as we just did, it's often more convenient to pass a list of layers when creating the `Sequential` model. You can also drop the `InputLayer` and instead specify the `input_shape` in the first layer:

```
model = tf.keras.Sequential([
    tf.keras.layers.Flatten(input_shape=[28, 28]),
    tf.keras.layers.Dense(300, activation="relu"),
    tf.keras.layers.Dense(100, activation="relu"),
    tf.keras.layers.Dense(10, activation="softmax")
])
```

The model's `summary()` method displays all the model's layers,[13] including each layer's name (which is automatically generated unless you set it when creating the layer), its output shape (`None` means the batch size can be anything), and its number of parameters. The summary ends with the total number of parameters, including trainable and non-trainable parameters. Here we only have trainable parameters (we will see some non-trainable parameters later in this chapter):

```
>>> model.summary()
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 flatten (Flatten)           (None, 784)               0

 dense (Dense)               (None, 300)               235500

 dense_1 (Dense)             (None, 100)               30100

 dense_2 (Dense)             (None, 10)                1010

=================================================================
Total params: 266,610
Trainable params: 266,610
Non-trainable params: 0
_________________________________________________________________
```

Note that `Dense` layers often have a *lot* of parameters. For example, the first hidden layer has 784 × 300 connection weights, plus 300 bias terms, which adds up to 235,500 parameters! This gives the model quite a lot of flexibility to fit the training data, but it also means that the model runs the risk of overfitting, especially when you do not have a lot of training data. We will come back to this later.

All layers in a model must have a unique name (e.g., “dense_2”). You can set the layer names explicitly using the constructor’s `name` argument, but generally it’s simpler to let Keras name the layers automatically, as we just did: Keras takes the layer’s class name and converts it to snake case (e.g., a layer from the `MyCoolLayer` class is named `"my_cool_layer"` by default). Moreover, Keras ensures that the name is globally unique, even across models, by appending an index if needed, as in `"dense_2"`. But why, I hear you ask, does it bother making the names unique across models? Well, this makes it possible to merge models easily without getting name conflicts.

> **TIP**
>
> All global state managed by Keras is stored in a *Keras session*, which you can clear using `tf.keras.backend.clear_session()`. In particular, this resets the name counters.

You can easily get a model's list of layers using the `layers` attribute, or use the `get_layer()` method to access a layer by name:

```
>>> model.layers
[<keras.layers.core.flatten.Flatten at 0x7fa1dea02250>,
 <keras.layers.core.dense.Dense at 0x7fa1c8f42520>,
 <keras.layers.core.dense.Dense at 0x7fa188be7ac0>,
 <keras.layers.core.dense.Dense at 0x7fa188be7fa0>]
>>> hidden1 = model.layers[1]
>>> hidden1.name
'dense'
>>> model.get_layer('dense') is hidden1
True
```

All the parameters of a layer can be accessed using its `get_weights()` and `set_weights()` methods. For a `Dense` layer, this includes both the connection weights and the bias terms:

```
>>> weights, biases = hidden1.get_weights()
>>> weights
array([[ 0.02448617, -0.00877795, -0.02189048, ...,  0.03859074,
-0.06889391],
       [ 0.00476504, -0.03105379, -0.0586676 , ..., -0.02763776,
-0.04165364],
       ...,
       [ 0.07061854, -0.06960931,  0.07038955, ..., 0.00034875,
0.02878492],
       [-0.06022581,  0.01577859, -0.02585464, ..., 0.00272203,
-0.06793761]],
       dtype=float32)
>>> weights.shape
```

```
(784, 300)
>>> biases
array([0., 0., 0., 0., 0., 0., 0., 0., 0., ...,  0., 0., 0.],
dtype=float32)
>>> biases.shape
(300,)
```

Notice that the `Dense` layer initialized the connection weights randomly (which is needed to break symmetry, as we discussed earlier), and the biases were initialized to zeros, which is fine. If you ever want to use a different initialization method, you can set `kernel_initializer` (*kernel* is another name for the matrix of connection weights) or `bias_initializer` when creating the layer. We will discuss initializers further in Chapter 11, but if you want the full list, see *https://keras.io/api/layers/initializers/*.

> **NOTE**
>
> The shape of the weight matrix depends on the number of inputs, which is why we specified the `input_shape` when creating the model. If you do not specify the input shape, it's OK: Keras will simply wait until it knows the input shape before it actually builds the model parameters. This will happen either when you feed it some data (e.g., during training), or when you call its `build()` method. Until the model parameters are built, you will not be able to do certain things, such as display the model summary or save the model. So, if you know the input shape when creating the model, it is best to specify it.

Compiling the model

After a model is created, you must call its `compile()` method to specify the loss function and the optimizer to use. Optionally, you can specify a list of extra metrics to compute during training and evaluation:

```
model.compile(loss="sparse_categorical_crossentropy",
              optimizer="sgd",
              metrics=["accuracy"])
```

> **NOTE**
>
> Using `loss="sparse_categorical_crossentropy"` is equivalent to using `loss=tf.keras.losses.sparse_categorical_crossentropy`. Similarly, specifying `optimizer="sgd"` is equivalent to specifying `optimizer=tf.keras.optimizers.SGD()`, and `metrics=["accuracy"]` is equivalent to `metrics=[tf.keras.metrics.sparse_categorical_accuracy]` (when using this loss). We will use many other losses, optimizers, and metrics in this book; for the full lists, see *https://keras.io/api/losses/*, *https://keras.io/api/optimizers/*, and *https://keras.io/api/metrics/*.

This code requires some explanation. First, we use the `"sparse_categorical_crossentropy"` loss because we have sparse labels (i.e., for each instance, there is just a target class index, from 0 to 9 in this case), and the classes are exclusive. If instead we had one target probability per class for each instance (such as one-hot vectors, e.g. `[0., 0., 0., 1., 0., 0., 0., 0., 0., 0.]` to represent class 3), then we would need to use the `"categorical_crossentropy"` loss instead. If we were doing binary classification or multilabel binary classification, then we would use the `"sigmoid"` activation function in the output layer instead of the `"softmax"` activation function, and we would use the `"binary_crossentropy"` loss.

> **TIP**
>
> If you want to convert sparse labels (i.e., class indices) to one-hot vector labels, use the `tf.keras.utils.to_categorical()` function. To go the other way round, use the `np.argmax()` function with `axis=1`.

Regarding the optimizer, `"sgd"` means that we will train the model using Stochastic Gradient Descent. In other words, Keras will perform the backpropagation algorithm described earlier (i.e., reverse-mode autodiff plus Gradient Descent). We will discuss more efficient optimizers in Chapter 11. They improve Gradient Descent, not autodiff.

> **NOTE**
>
> When using the `SGD` optimizer, it is important to tune the learning rate. So, you will generally want to use `optimizer=tf.keras.optimizers.SGD(learning_rate=???)` to set the learning rate, rather than `optimizer="sgd"`, which defaults to a learning rate of 0.01.

Finally, since this is a classifier, it's useful to measure its accuracy during training and evaluation, which is why we set `metrics=["accuracy"]`.

Training and evaluating the model

Now the model is ready to be trained. For this we simply need to call its `fit()` method:

```
>>> history = model.fit(X_train, y_train, epochs=30,
...                     validation_data=(X_valid, y_valid))
...
Epoch 1/30
1719/1719 [==============================] - 2s 989us/step
  - loss: 0.7220 - sparse_categorical_accuracy: 0.7649
  - val_loss: 0.4959 - val_sparse_categorical_accuracy: 0.8332
Epoch 2/30
1719/1719 [==============================] - 2s 964us/step
  - loss: 0.4825 - sparse_categorical_accuracy: 0.8332
  - val_loss: 0.4567 - val_sparse_categorical_accuracy: 0.8384
[...]
Epoch 30/30
1719/1719 [==============================] - 2s 963us/step
  - loss: 0.2235 - sparse_categorical_accuracy: 0.9200
  - val_loss: 0.3056 - val_sparse_categorical_accuracy: 0.8894
```

We pass it the input features (`X_train`) and the target classes (`y_train`), as well as the number of epochs to train (or else it would default to just 1, which would definitely not be enough to converge to a good solution). We also pass a validation set (this is optional). Keras will measure the loss and the extra metrics on this set at the end of each epoch, which is very useful to see how well the model really performs. If the performance on the training set is much better than on the validation set, your model is probably overfitting the training set, or there is a bug, such as a data mismatch between the training set and the validation set.

> **TIP**
>
> Shape errors are quite common, especially when getting started, so you should familiarize yourself with the error messages: try fitting a model with inputs and/or labels of the wrong shape, and see the errors you get. Similarly, try compiling the model with `loss="categorical_crossentropy"` instead of `loss="sparse_categorical_crossentropy"`, or remove the `Flatten` layer.

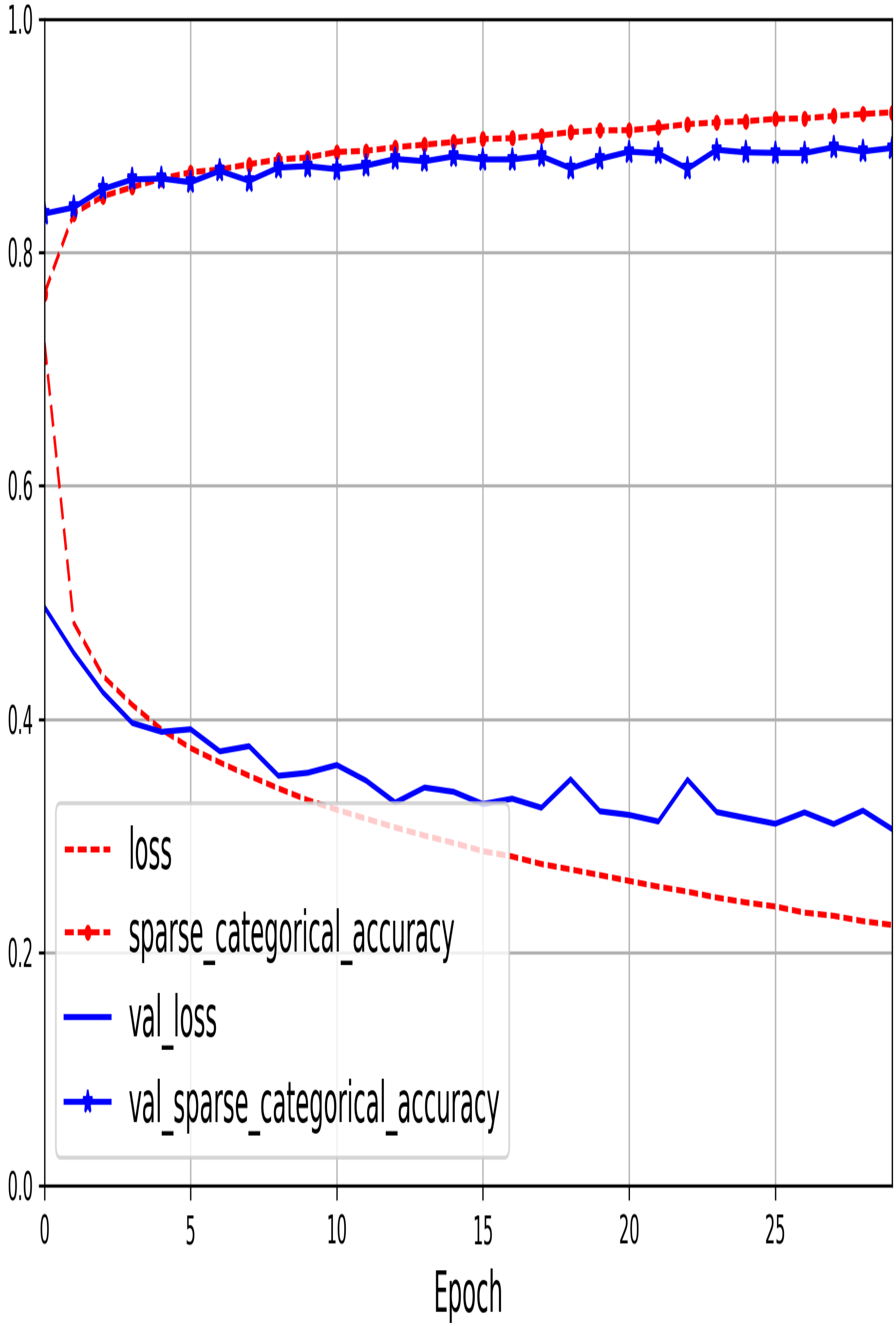
And that's it! The neural network is trained. At each epoch during training, Keras displays the number of mini-batches processed so far, on the left side of the progress bar. The batch size is 32 by default, and since the training set has 55,000 images, the model goes through 1,719 batches per epoch: 1,718 of size 32, and one of size 24. After the progress bar, you can see the mean training time per sample, and the loss and accuracy (or any other extra metrics you asked for) on both the training set and the validation set. Notice that the training loss went down, which is a good sign, and the validation accuracy reached 88.94% after 30 epochs. That's slightly below the training accuracy, so there is a little bit of overfitting going on, but not a huge amount.

> **TIP**
>
> Instead of passing a validation set using the `validation_data` argument, you could set `validation_split` to the ratio of the training set that you want Keras to use for validation. For example, `validation_split=0.1` tells Keras to use the last 10% of the data (before shuffling) for validation.

If the training set was very skewed, with some classes being overrepresented and others underrepresented, it would be useful to set the `class_weight` argument when calling the `fit()` method, to give a larger weight to underrepresented classes and a lower weight to overrepresented classes. These weights would be used by Keras when computing the loss. If you need per-instance weights, set the `sample_weight` argument. If both `class_weight` and `sample_weight` are provided, then Keras multiplies them. Per-instance weights could be useful for example if some instances were labeled by experts while others were labeled using a crowdsourcing platform: you might want to give more weight to the former. You can also provide sample weights (but not class weights) for the validation set by adding them as a third item in the `validation_data` tuple.

The `fit()` method returns a `History` object containing the training parameters (`history.params`), the list of epochs it went through (`history.epoch`), and most importantly a dictionary (`history.history`) containing the loss and extra metrics it measured at the end of each epoch on the training set and on the validation set (if any). If you use this dictionary to create a Pandas DataFrame and call its `plot()` method, you get the learning curves shown in Figure 10-11:

```
import matplotlib.pyplot as plt
import pandas as pd

pd.DataFrame(history.history).plot(
    figsize=(8, 5), xlim=[0, 29], ylim=[0, 1], grid=True,
xlabel="Epoch",
    style=["r--", "r--.", "b-", "b-*"])
plt.show()
```



1.0
0.8
0.6
0.4
0.2
0.0
0
5
10
15
20
25
Epoch
loss
sparse_categorical_accuracy
val_loss
val_sparse_categorical_accuracy

Figure 10-11. Learning curves: the mean training loss and accuracy measured over each epoch, and the mean validation loss and accuracy measured at the end of each epoch

You can see that both the training accuracy and the validation accuracy steadily increase during training, while the training loss and the validation loss decrease. Good! The validation curves are relatively close to each other at first, but they get further apart over time, which shows that there's a little bit of overfitting. In this particular case, the model looks like it performed better on the validation set than on the training set at the beginning of training. But that's not the case: indeed, the validation error is computed at the *end* of each epoch, while the training error is computed using a running mean *during* each epoch. So the training curve should be shifted by half an epoch to the left. If you do that, you will see that the training and validation curves overlap almost perfectly at the beginning of training.

> **TIP**
>
> When plotting the training curve, it should be shifted by half an epoch to the left.

The training set performance ends up beating the validation performance, as is generally the case when you train for long enough. You can tell that the model has not quite converged yet, as the validation loss is still going down, so you should probably continue training. It's as simple as calling the `fit()` method again, since Keras just continues training where it left off: you should be able to reach about 89.8% validation accuracy, while the training accuracy will continue to rise up to 100% (this is not always the case).

If you are not satisfied with the performance of your model, you should go back and tune the hyperparameters. The first one to check is the learning rate. If that doesn't help, try another optimizer (and always retune the learning rate after changing any hyperparameter). If the performance is still not great, then try tuning model hyperparameters such as the number of layers, the number of neurons per layer, and the types of activation functions to use for each hidden layer. You can also try tuning other hyperparameters, such as the batch size (it can be set in the `fit()` method using the `batch_size` argument, which defaults to 32). We will get back to hyperparameter tuning at the end of this chapter. Once you are satisfied with your model's validation accuracy, you should evaluate it on the test set to estimate the generalization error before you deploy the model to production. You can easily do this using the `evaluate()` method (it also supports several other arguments, such as `batch_size` and `sample_weight`; please check the documentation for more details):

```
>>> model.evaluate(X_test, y_test)
313/313 [==============================] - 0s 626us/step
  - loss: 0.3243 - sparse_categorical_accuracy: 0.8864
[0.32431697845458984, 0.8863999843597412]
```

As we saw in Chapter 2, it is common to get slightly lower performance on the test set than on the validation set, because the hyperparameters are tuned on the validation set, not the test set (however, in this example, we did not do any hyperparameter tuning, so the lower accuracy is just bad luck). Remember to resist the temptation to tweak the hyperparameters on the test set, or else your estimate of the generalization error will be too optimistic.

Using the model to make predictions

Next, we can use the model's `predict()` method to make predictions on new instances. Since we don't have actual new instances, we will just use the first three instances of the test set:

```
>>> X_new = X_test[:3]
>>> y_proba = model.predict(X_new)
>>> y_proba.round(2)
array([[0.  , 0.  , 0.  , 0.  , 0.  , 0.01, 0.  , 0.02, 0.  ,
0.97],
       [0.  , 0.  , 0.99, 0.  , 0.01, 0.  , 0.  , 0.  , 0.  , 0.
],
       [0.  , 1.  , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  , 0.
]],
      dtype=float32)
```

As you can see, for each instance the model estimates one probability per class, from class 0 to class 9. This is similar to the output of the `predict_proba()` method in Scikit-Learn classifiers. For example, for the first image it estimates that the probability of class 9 (ankle boot) is 96%, the probability of class 7 (sneaker) is 2%, the probability of class 5 (sandal) is 1%, and the probabilities of the other classes are negligible. In other words, it is highly confident that the first image is footwear, most likely ankle boots but possibly sneakers or sandals. If you only care about the class with the highest estimated probability (even if that probability is quite low), then you can use the `argmax()` to get the highest probability class index for each instance:

```
>>> import numpy as np
>>> y_pred = y_proba.argmax(axis=-1)
>>> y_pred
array([9, 2, 1])
>>> np.array(class_names)[y_pred]
array(['Ankle boot', 'Pullover', 'Trouser'], dtype='<U11')
```

Here, the classifier actually classified all three images correctly (these images are shown in Figure 10-12):

```
>>> y_new = y_test[:3]
>>> y_new
array([9, 2, 1], dtype=uint8)
```

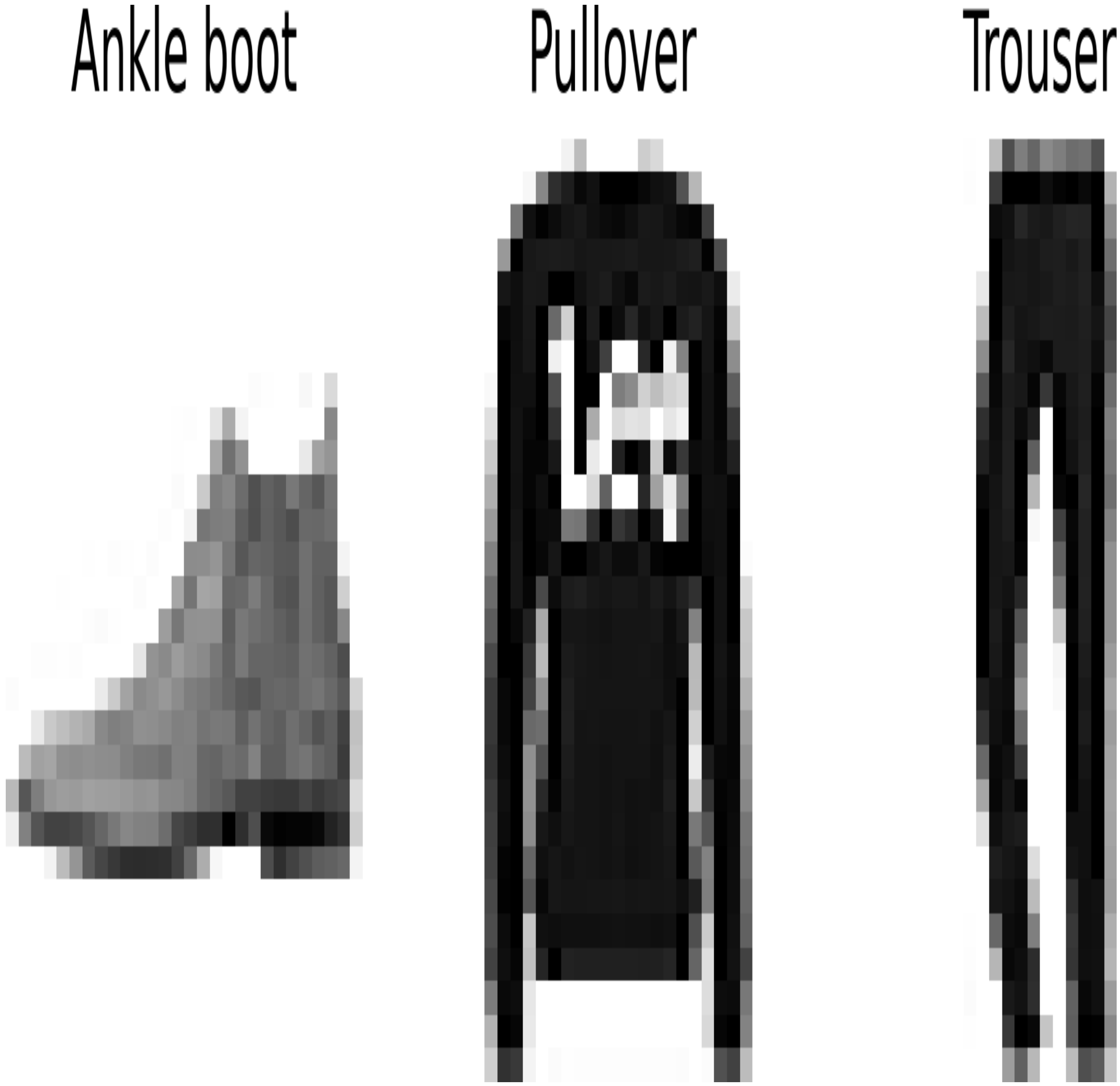


Figure 10-12. Correctly classified Fashion MNIST images

Now you know how to use the Sequential API to build, train, evaluate, and use a classification MLP. But what about regression?

Building a Regression MLP Using the Sequential API

Let's switch back to the California housing problem and tackle it using the same MLP as earlier, with 3 hidden layers composed of 50 neurons each, but this time building it with Keras.

Using the Sequential API to build, train, evaluate, and use a regression MLP is quite similar to what we did for classification. The main differences in the following code example are the fact that the output layer has a single neuron (since we only want to predict a single value) and it uses no activation function, the loss function is the mean squared error, the metric is the RMSE, and we're using an Adam optimizer like Scikit-Learn's `MLPRegressor` did. Moreover, in this example we don't need a `Flatten` layer, and instead we're using a `Normalization` layer as the first layer: it does the same thing as Scikit-Learn's `StandardScaler`, but it must be fitted to the training data using its `adapt()` method *before* you call the model's `fit()` method. Keras has other preprocessing layers which will be covered in Chapter 13.

```
tf.random.set_seed(42)
norm_layer =
tf.keras.layers.Normalization(input_shape=X_train.shape[1:])
model = tf.keras.Sequential([
    norm_layer,
    tf.keras.layers.Dense(50, activation="relu"),
    tf.keras.layers.Dense(50, activation="relu"),
    tf.keras.layers.Dense(50, activation="relu"),
    tf.keras.layers.Dense(1)
])
optimizer = tf.keras.optimizers.Adam(learning_rate=1e-3)
model.compile(loss="mse", optimizer=optimizer, metrics=
["RootMeanSquaredError"])
norm_layer.adapt(X_train)
history = model.fit(X_train, y_train, epochs=20,
                    validation_data=(X_valid, y_valid))
mse_test, rmse_test = model.evaluate(X_test, y_test)
X_new = X_test[:3]
y_pred = model.predict(X_new)
```

NOTE

The `Normalization` layer learns the feature means and standard deviations in the training data when you call the `adapt()` method. Yet when you display the model's summary, these statistics are listed as non-trainable. This is because these parameters are not affected by Gradient Descent.

As you can see, the Sequential API is quite clean and straightforward. However, although `Sequential` models are extremely common, it is sometimes useful to build neural networks with more complex topologies, or with multiple inputs or outputs. For this purpose, Keras offers the Functional API.

Building Complex Models Using the Functional API

One example of a nonsequential neural network is a *Wide & Deep* neural network. This neural network architecture was introduced in a 2016 paper by Heng-Tze Cheng et al.[14] It connects all or part of the inputs directly to the output layer, as shown in Figure 10-13. This architecture makes it possible for the neural network to learn both deep patterns (using the deep path) and simple rules (through the short path).[15] In contrast, a regular MLP forces all the data to flow through the full stack of layers; thus, simple patterns in the data may end up being distorted by this sequence of transformations.

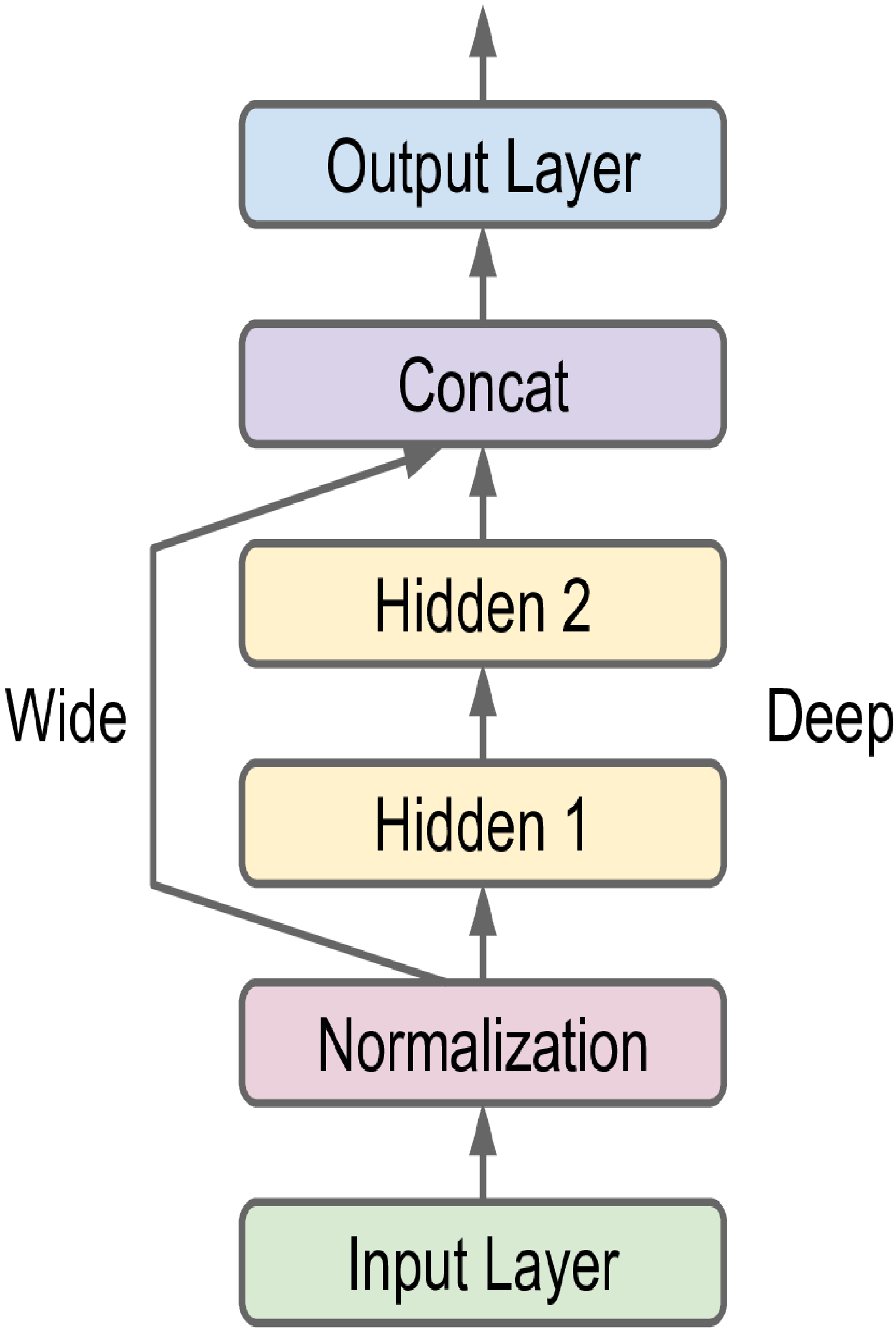

Output Layer
Concat
Wide
Hidden 2
Deep
Hidden 1
Normalization
Input Layer

Figure 10-13. Wide & Deep neural network

Let's build such a neural network to tackle the California housing problem:

```
normalization_layer = tf.keras.layers.Normalization()
hidden_layer1 = tf.keras.layers.Dense(30, activation="relu")
hidden_layer2 = tf.keras.layers.Dense(30, activation="relu")
concat_layer = tf.keras.layers.Concatenate()
output_layer = tf.keras.layers.Dense(1)

input_ = tf.keras.layers.Input(shape=X_train.shape[1:])
normalized = normalization_layer(input_)
hidden1 = hidden_layer1(normalized)
hidden2 = hidden_layer2(hidden1)
concat = concat_layer([input_, hidden2])
output = output_layer(concat)

model = tf.keras.Model(inputs=[input_], outputs=[output])
```

At a high level, the first five lines create all the layers we need to build the model, the next six lines use these layers just like functions to go from the input to the output, and the last line creates a Keras `Model` object by pointing to the input and the output. Let's go through this code in more details:

- First, we create five layers: a `Normalization` layer to standardize the inputs, two `Dense` layers with 30 neurons each, using the ReLU activation function, a `Concatenate` layer, and one more `Dense` layer with a single neuron for the output layer, without any activation function.

- Next, we create an `Input` object (the variable name `input_` is used to avoid overshadowing Python's built-in `input()` function). This is a specification of the kind of input the model will get, including its `shape` and optionally its `dtype`, which defaults to 32-bit floats. A model may actually have multiple inputs, as we will see shortly.

- Then we use the `Normalization` layer just like a function, passing it the `Input` object. This is why this is called the Functional API. Note that we are just telling Keras how it should connect the layers together; no actual data is being processed yet, as the `Input` object is just a data specification. In other words, it's a symbolic input. The output of this call is also symbolic: `normalized` doesn't store any actual data, it's just used to construct the model.

- In the same may, we then pass `normalized` to `hidden_layer1`, which outputs `hidden1`, and we pass `hidden1` to `hidden_layer2`, which outputs `hidden2`.

- So far, we've connected the layers sequentially, but then we use the `concat_layer` to concatenate the input and the second hidden layer's output. Again, no actual data is concatenated yet: it's all symbolic, to build the model.

- Then we pass `concat` to the `output_layer`, which gives us the final `output`.

- Lastly, we create a Keras `Model`, specifying which inputs and outputs to use.

Once you have built this Keras model, everything is exactly like earlier, so there's no need to repeat it here: you must compile the model, adapt the `Normalization` layer, fit the model, evaluate it, and use it to make predictions.

But what if you want to send a subset of the features through the wide path and a different subset (possibly overlapping) through the deep path (see Figure 10-14)? In this case, one solution is to use multiple inputs. For example, suppose we want to send five features through the wide path (features 0 to 4), and six features through the deep path (features 2 to 7):

```
input_wide = tf.keras.layers.Input(shape=[5])  # features 0 to 4
input_deep = tf.keras.layers.Input(shape=[6])  # features 2 to 7
```

```
norm_layer_wide = tf.keras.layers.Normalization()
norm_layer_deep = tf.keras.layers.Normalization()
norm_wide = norm_layer_wide(input_wide)
norm_deep = norm_layer_deep(input_deep)
hidden1 = tf.keras.layers.Dense(30, activation="relu")(norm_deep)
hidden2 = tf.keras.layers.Dense(30, activation="relu")(hidden1)
concat = tf.keras.layers.concatenate([norm_wide, hidden2])
output = tf.keras.layers.Dense(1)(concat)
model = tf.keras.Model(inputs=[input_wide, input_deep], outputs=
[output])
```

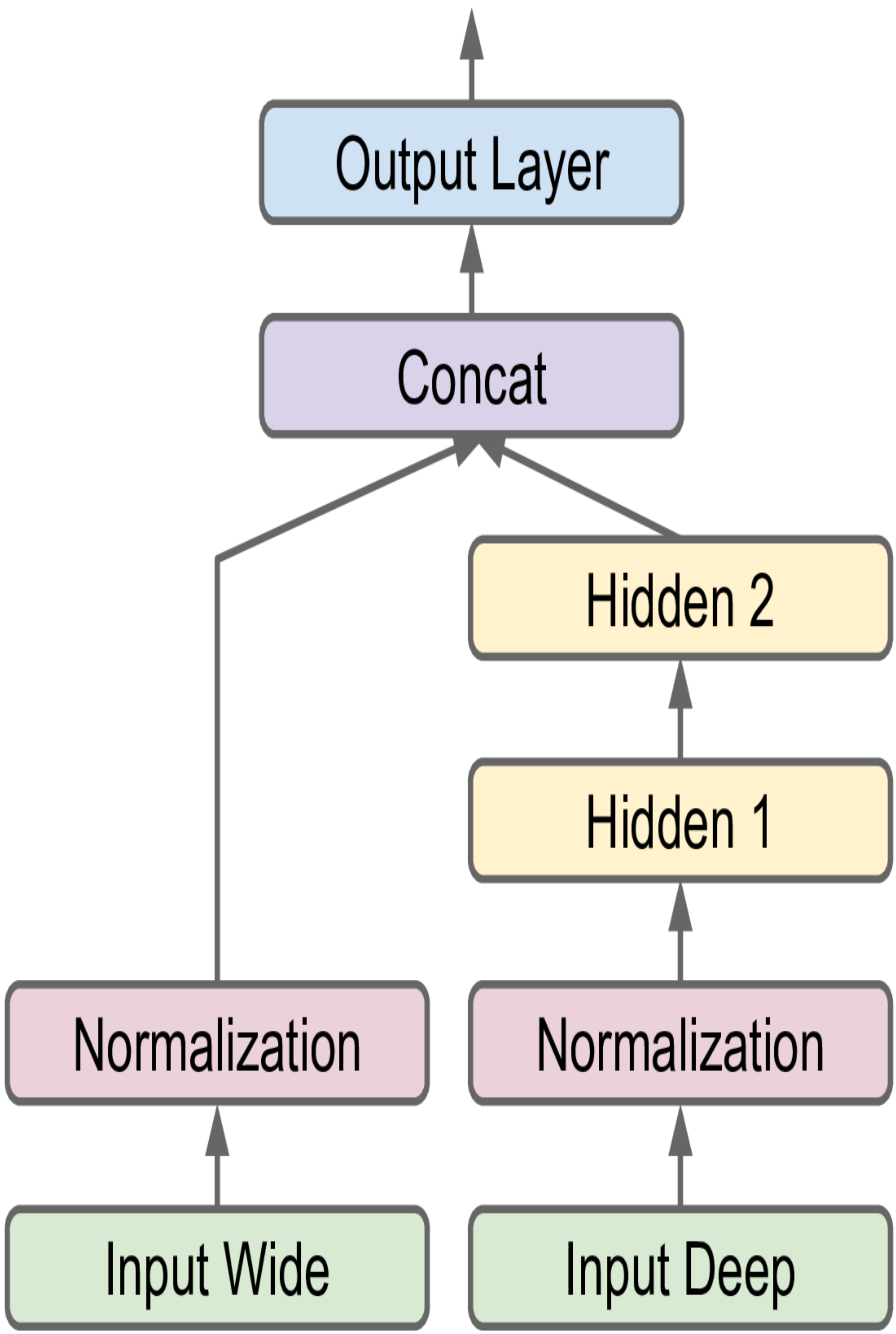

Output Layer
Concat
Hidden 2
Hidden 1
Normalization
Normalization
Input Wide
Input Deep

Figure 10-14. Handling multiple inputs

There are a few things to note in this code example, compared to the previous example:

- Each `Dense` layer is created and called on the same line. This is a common practice, as it makes the code more concise without losing clarity. However, we can't do this with the `Normalization` layer since we need a reference to the layer to be able to call its `adapt()` method before fitting the model.
- We used `tf.keras.layers.concatenate()`, which creates a `Concatenate` layer and calls it with the given inputs.
- We specified `inputs=[input_wide, input_deep]` when creating the model, since there are two inputs.

Now we can compile the model as usual, but when we call the `fit()` method, instead of passing a single input matrix `X_train`, we must pass a pair of matrices `(X_train_wide, X_train_deep)`: one per input. The same is true for `X_valid`, and also for `X_test` and `X_new` when you call `evaluate()` or `predict()`:

```
optimizer = tf.keras.optimizers.Adam(learning_rate=1e-3)
model.compile(loss="mse", optimizer=optimizer, metrics=
["RootMeanSquaredError"])

X_train_wide, X_train_deep = X_train[:, :5], X_train[:, 2:]
X_valid_wide, X_valid_deep = X_valid[:, :5], X_valid[:, 2:]
X_test_wide, X_test_deep = X_test[:, :5], X_test[:, 2:]
X_new_wide, X_new_deep = X_test_wide[:3], X_test_deep[:3]

norm_layer_wide.adapt(X_train_wide)
norm_layer_deep.adapt(X_train_deep)
history = model.fit((X_train_wide, X_train_deep), y_train,
epochs=20,
                    validation_data=((X_valid_wide,
X_valid_deep), y_valid))
mse_test = model.evaluate((X_test_wide, X_test_deep), y_test)
y_pred = model.predict((X_new_wide, X_new_deep))
```

> **TIP**
>
> Instead of passing a tuple `(X_train_wide, X_train_deep)`, you can pass a dictionary `{"input_wide": X_train_wide, "input_deep": X_train_deep}`, assuming you set `name="input_wide"` and `name="input_deep"` when creating the inputs. This is highly recommended when there are many inputs, to clarify the code and avoid getting the order wrong.

There are also many use cases in which you may want to have multiple outputs:

- The task may demand it. For instance, you may want to locate and classify the main object in a picture. This is both a regression tasks and a classification task.
- Similarly, you may have multiple independent tasks based on the same data. Sure, you could train one neural network per task, but in many cases you will get better results on all tasks by training a single neural network with one output per task. This is because the neural network can learn features in the data that are useful across tasks. For example, you could perform *multitask classification* on pictures of faces, using one output to classify the person's facial expression (smiling, surprised, etc.) and another output to identify whether they are wearing glasses or not.
- Another use case is as a regularization technique (i.e., a training constraint whose objective is to reduce overfitting and thus improve the model's ability to generalize). For example, you may want to add an auxiliary output in a neural network architecture (see Figure 10-15) to ensure that the underlying part of the network learns something useful on its own, without relying on the rest of the network.

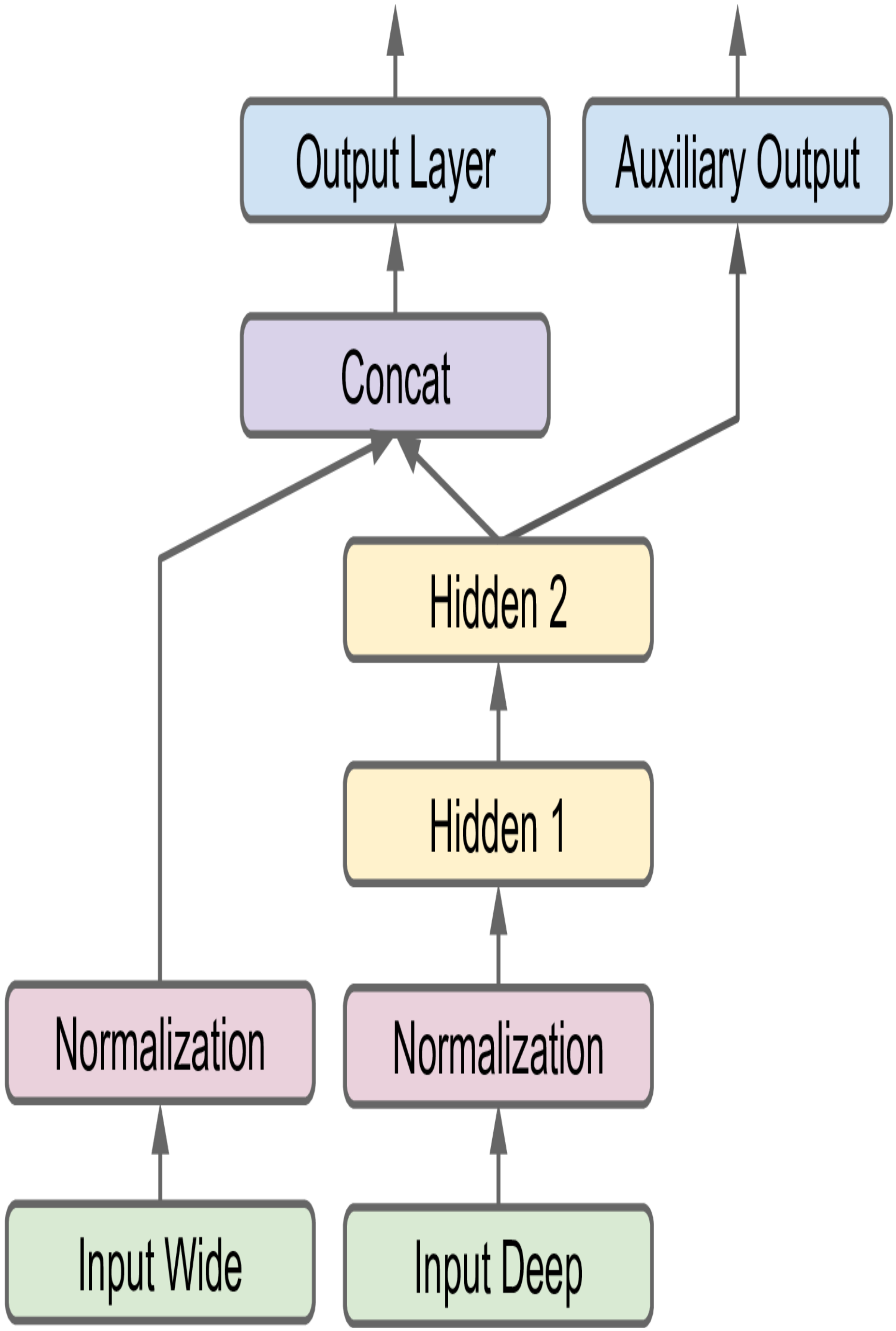

Output Layer
Auxiliary Output
Concat
Hidden 2
Hidden 1
Normalization
Normalization
Input Wide
Input Deep

Figure 10-15. Handling multiple outputs, in this example to add an auxiliary output for regularization

Adding an extra output is quite easy: just connect it to the appropriate layer and add it to your model's list of outputs. For example, the following code builds the network represented in Figure 10-15:

```
[...]  # Same as above, up to the main output layer
output = tf.keras.layers.Dense(1)(concat)
aux_output = tf.keras.layers.Dense(1)(hidden2)
model = tf.keras.Model(inputs=[input_wide, input_deep],
                       outputs=[output, aux_output])
```

Each output will need its own loss function. Therefore, when we compile the model, we should pass a list of losses. If we pass a single loss, Keras will assume that the same loss must be used for all outputs. By default, Keras will compute all the losses and simply add them up to get the final loss used for training. Since we care much more about the main output than about the auxiliary output (as it is just used for regularization), we want to give the main output's loss a much greater weight. Luckily, it is possible to set all the loss weights when compiling the model:

```
optimizer = tf.keras.optimizers.Adam(learning_rate=1e-3)
model.compile(loss=("mse", "mse"), loss_weights=(0.9, 0.1),
optimizer=optimizer,
              metrics=["RootMeanSquaredError"])
```

TIP

Instead of passing a tuple `loss=("mse", "mse")`, you can pass a dictionary `loss={"output": "mse", "aux_output": "mse"}`, assuming you created the output layers with `name="output"` and `name="aux_output"`. Just like for the inputs, this clarifies the code and avoids errors when there are several outputs. You can also pass a dictionary for `loss_weights`.

Now when you train the model, you need to provide labels for each output. In this example, the main output and the auxiliary output should try to predict the same thing, so they should use the same labels. So instead of passing `y_train`, you need to pass `(y_train, y_train)`, or a dictionary `{"output": y_train, "aux_output": y_train}` if the outputs were named `"output"` and `"aux_output"`. The same goes for `y_valid` and `y_test`:

```
norm_layer_wide.adapt(X_train_wide)
norm_layer_deep.adapt(X_train_deep)
history = model.fit(
    (X_train_wide, X_train_deep), (y_train, y_train), epochs=20,
    validation_data=((X_valid_wide, X_valid_deep), (y_valid,
y_valid))
)
```

When you evaluate the model, Keras returns the weighted sum of the losses, as well as all the individual losses and metrics:

```
eval_results = model.evaluate((X_test_wide, X_test_deep),
(y_test, y_test))
weighted_sum_of_losses, main_loss, aux_loss, main_rmse, aux_rmse
= eval_results
```

TIP

If you set `return_dict=True`, then `evaluate()` will return a dictionary instead of a big tuple.

Similarly, the `predict()` method will return predictions for each output:

```
y_pred_main, y_pred_aux = model.predict((X_new_wide, X_new_deep))
```

The `predict()` method returns a tuple, and it does not have a `return_dict` argument to get a dictionary instead, but you can create one using `model.output_names`:

```
y_pred_tuple = model.predict((X_new_wide, X_new_deep))
y_pred = dict(zip(model.output_names, y_pred_tuple))
```

As you can see, you can build all sorts of architectures with the Functional API. Let's look at one last way you can build Keras models.

Using the Subclassing API to Build Dynamic Models

Both the Sequential API and the Functional API are declarative: you start by declaring which layers you want to use and how they should be connected, and only then can you start feeding the model some data for training or inference. This has many advantages: the model can easily be saved, cloned, and shared; its structure can be displayed and analyzed; the framework can infer shapes and check types, so errors can be caught early (i.e., before any data ever goes through the model). It's also fairly straightforward to debug, since the whole model is a static graph of layers. But the flip side is just that: it's static. Some models involve loops, varying shapes, conditional branching, and other dynamic behaviors. For such cases, or simply if you prefer a more imperative programming style, the Subclassing API is for you.

You must subclass the `Model` class, create the layers you need in the constructor, and use them to perform the computations you want in the `call()` method. For example, creating an instance of the following `WideAndDeepModel` class gives us an equivalent model to the one we just built with the Functional API:

```
class WideAndDeepModel(tf.keras.Model):
    def __init__(self, units=30, activation="relu", **kwargs):
        super().__init__(**kwargs)  # needed to support naming
the model
        self.norm_layer_wide = tf.keras.layers.Normalization()
        self.norm_layer_deep = tf.keras.layers.Normalization()
        self.hidden1 = tf.keras.layers.Dense(units,
activation=activation)
        self.hidden2 = tf.keras.layers.Dense(units,
activation=activation)
        self.main_output = tf.keras.layers.Dense(1)
        self.aux_output = tf.keras.layers.Dense(1)

    def call(self, inputs):
        input_wide, input_deep = inputs
```

```
        norm_wide = self.norm_layer_wide(input_wide)
        norm_deep = self.norm_layer_deep(input_deep)
        hidden1 = self.hidden1(norm_deep)
        hidden2 = self.hidden2(hidden1)
        concat = tf.keras.layers.concatenate([norm_wide,
hidden2])
        output = self.main_output(concat)
        aux_output = self.aux_output(hidden2)
        return output, aux_output

model = WideAndDeepModel(30, activation="relu",
name="my_cool_model")
```

This example looks very much like the Functional API, except we separate the creation of the layers[16] in the constructor from their usage in the `call()` method. We also do not need to create the `Input` objects: we just use the `input` argument to the `call()` method.

Now that you have a model instance, you can compile it, adapt its normalization layers (e.g., using `model.norm_layer_wide.adapt(...)` and `model.norm_layer_deep.adapt(...)`), fit it, evaluate it, and use it to make predictions, exactly like you did with the Functional API.

The big difference with this API is that you can do pretty much anything you want in the `call()` method: `for` loops, `if` statements, low-level TensorFlow operations—your imagination is the limit (see Chapter 12)! This makes it a great API when experimenting with new ideas, especially for researchers. However, this extra flexibility does come at a cost: your model's architecture is hidden within the `call()` method, so Keras cannot easily inspect it, the model cannot be cloned using `tf.keras.models.clone_model()`, and when you call the `summary()` method, you only get a list of layers, without any information on how they are connected to each other. Moreover, Keras cannot check types and shapes ahead of time, and it is easier to make mistakes. So unless you really need that extra flexibility, you should probably stick to the Sequential API or the Functional API.

> **TIP**
>
> Keras models can be used just like regular layers, so you can easily combine them to build complex architectures.

Now that you know how to build and train neural nets using Keras, you will want to save them!

Saving and Restoring a Model

Saving a trained Keras model is as simple as it gets:

```
model.save("my_keras_model")
```

By default, Keras saves the model using TensorFlow's *SavedModel* format: this is a directory (with the given name) containing several files and subdirectories. In particular, the `saved_model.pb` file contains the model's architecture and logic in the form of a serialized computation graph, so you don't need to deploy the model's source code in order to use it in production, the SavedModel is sufficient (we will see how this works in Chapter 12). The `keras_metadata.pb` file contains extra information needed by Keras. The `variables` subdirectory contains all the parameter values (including the connection weights, the biases, the normalization statistics, and the optimizer's parameters), possibly split across multiple files if the model is very large. Lastly, the `assets` directory may contain extra files, for example data samples, feature names, class names, and so on. By default, the `assets` directory is empty. Since the optimizer is also saved, including its hyperparameters and any state it may have, after loading the model you can continue training if you want.

> **NOTE**
>
> If you set `save_format="h5"` or use a name ending with `.h5`, then Keras will save the model to a single file using the HDF5 format. However, this format does not support the Subclassing API, and most TensorFlow deployment tools require the SavedModel format.

You will typically have a script that trains a model and saves it, and one or more scripts (or web services) that load the model and use it to evaluate it or to make predictions. Loading the model is just as easy as saving it:

```
model = tf.keras.models.load_model("my_keras_model")
y_pred_main, y_pred_aux = model.predict((X_new_wide, X_new_deep))
```

You can also use `save_weights()` and `load_weights()` to save and load only the parameter values. This includes the connection weights, biases, preprocessing stats, optimizer state, etc. The parameter values are saved in one or more files such as `my_weights.data-00004-of-00052`, plus an index file like `my_weights.index`.

Saving just the weights is faster and uses less disk space than saving the whole model, so it's perfect to save quick checkpoints during training. If you're training a big model, and it takes hours or days, then you must save checkpoints regularly in case the computer crashes. But how can you tell the `fit()` method to save checkpoints? Use callbacks.

Using Callbacks

The `fit()` method accepts a `callbacks` argument that lets you specify a list of objects that Keras will call before and after training, before and after each epoch, and even before and after processing each batch. For example, the `ModelCheckpoint` callback saves checkpoints of your model at regular intervals during training, by default at the end of each epoch:

```
checkpoint_cb =
tf.keras.callbacks.ModelCheckpoint("my_checkpoints",

save_weights_only=True)
history = model.fit([...], callbacks=[checkpoint_cb])
```

Moreover, if you use a validation set during training, you can set `save_best_only=True` when creating the `ModelCheckpoint`. In this case, it will only save your model when its performance on the validation set is the best so far. This way, you do not need to worry about training for too long and overfitting the training set: simply restore the last saved model after training, and this will be the best model on the validation set. This is one way to implement early stopping (introduced in Chapter 4), but it won't actually stop training.

Another way is to use the `EarlyStopping` callback. It will interrupt training when it measures no progress on the validation set for a number of epochs (defined by the `patience` argument), and if you set `restore_best_weights=True` it will roll back to the best model at the end of training. You can combine both callbacks to save checkpoints of your model in case your computer crashes, and interrupt training early when there is no more progress, to avoid wasting time and resources and to reduce overfitting:

```
early_stopping_cb = tf.keras.callbacks.EarlyStopping(patience=10,

restore_best_weights=True)
history = model.fit([...], callbacks=[checkpoint_cb,
early_stopping_cb])
```

The number of epochs can be set to a large value since training will stop automatically when there is no more progress (just make sure the learning rate is not too small, or else it might keep making slow progress until the end). The `EarlyStopping` callback will store the weights of the best model in RAM, and it will restore them for you at the end of training.

TIP

There are many other callbacks available in the `tf.keras.callbacks` package.

If you need extra control, you can easily write your own custom callbacks. For example, the following custom callback will display the ratio between the validation loss and the training loss during training (e.g., to detect overfitting):

```
class PrintValTrainRatioCallback(tf.keras.callbacks.Callback):
    def on_epoch_end(self, epoch, logs):
        ratio = logs["val_loss"] / logs["loss"]
        print(f"Epoch={epoch}, val/train={ratio:.2f}")
```

As you might expect, you can implement `on_train_begin()`, `on_train_end()`, `on_epoch_begin()`, `on_epoch_end()`, `on_batch_begin()`, and `on_batch_end()`. Callbacks can also be used during evaluation and predictions, should you ever need them (e.g., for debugging). For evaluation, you should implement `on_test_begin()`, `on_test_end()`, `on_test_batch_begin()`, or `on_test_batch_end()`, which are called by `evaluate()`. For prediction, you should implement `on_predict_begin()`, `on_predict_end()`, `on_predict_batch_begin()`, or `on_predict_batch_end()`, which are called by `predict()`.

Now let's take a look at one more tool you should definitely have in your toolbox when using Keras: TensorBoard.

Using TensorBoard for Visualization

TensorBoard is a great interactive visualization tool that you can use to view the learning curves during training, compare curves and metrics between multiple runs, visualize the computation graph, analyze training statistics, view images generated by your model, visualize complex multidimensional data projected down to 3D and automatically clustered for you, *profile* your network (i.e., measure its speed to identify bottlenecks), and more!

TensorBoard is installed automatically when you install TensorFlow. However, you will need a TensorBoard plugin to visualize profiling data. If you followed the installation instructions at *https://homl.info/install* to run everything locally, then you already have the plugin installed, but if you are using Colab, then you must run the following command:

```
%pip install -q -U tensorboard-plugin-profile
```

To use TensorBoard, you must modify your program so that it outputs the data you want to visualize to special binary log files called *event files*. Each binary data record is called a *summary*. The TensorBoard server will monitor the log directory, and it will automatically pick up the changes and update the visualizations: this allows you to visualize live data (with a short delay), such as the learning curves during training. In general, you want to point the TensorBoard server to a root log directory and configure your program so that it writes to a different subdirectory every time it runs. This way, the same TensorBoard server instance will allow you to visualize and compare data from multiple runs of your program, without getting everything mixed up.

Let's name the root log directory `my_logs`, and let's define a little function that generates the path of the log subdirectory based on the current date and time, so that it's different at every run:

```
from pathlib import Path
from time import strftime

def get_run_logdir(root_logdir="my_logs"):
    return Path(root_logdir) / strftime("run_%Y_%m_%d_%H_%M_%S")

run_logdir = get_run_logdir()  # e.g.,
my_logs/run_2022_08_01_17_25_59
```

The good news is that Keras provides a convenient `TensorBoard()` callback which will take care of creating the log directory for you (along with its parent directories if needed), and it will create event files and write summaries to them during training. It will measure your model's training and validation loss and metrics (in this case, the MSE and RMSE), and it will also profile your neural network. It is straightforward to use:

```
tensorboard_cb = tf.keras.callbacks.TensorBoard(run_logdir,
                                                 profile_batch=
(100, 200))
history = model.fit([...], callbacks=[tensorboard_cb])
```

And that's all there is to it! In this example, it will profile the network between batches 100 and 200 during the first epoch. Why 100 and 200? Well, it often takes a few batches for the neural network to "warm up", so you don't want to profile too early. And profiling uses a bit of resources, so it's best not to do it for every batch.

Next, try changing the learning rate from 0.001 to 0.002, and run the code again, with a new log subdirectory. You will end up with a directory structure similar to this one:

```
my_logs
├── run_2022_08_01_17_25_59
│   ├── train
│   │   ├──
events.out.tfevents.1659331561.my_host_name.42042.0.v2
│   │   ├── events.out.tfevents.1659331562.my_host_name.profile-
empty
│   │   └── plugins
│   │       └── profile
│   │           └── 2022_08_01_17_26_02
│   │               ├── my_host_name.input_pipeline.pb
│   │               └── [...]
│   └── validation
│       └──
events.out.tfevents.1659331562.my_host_name.42042.1.v2
└── run_2022_08_01_17_31_12
    └── [...]
```

There's one directory per run, each containing one subdirectory for training logs and one for validation logs. Both contain event files, and the training logs also include profiling traces.

Now that you have the event files ready, it's time to start the TensorBoard server. This can be done directly within Jupyter or Colab using the Jupyter extension for TensorBoard, which gets installed along with the TensorBoard library. This extension is preinstalled in Colab. The following code loads the Jupyter extension for TensorBoard, and the second line starts a TensorBoard server for the `my_logs` directory, and it connects to this server and displays the user interface directly inside of Jupyter. The server listens on the first available TCP port greater or equal to 6006 (or you can set the port you want using the `--port` option).

```
%load_ext tensorboard
%tensorboard --logdir=./my_logs
```

TIP

If you are running everything on your own machine, it's also possible to start TensorBoard by executing `tensorboard --logdir=./my_logs` in a terminal. You must first activate the conda environment in which you installed TensorBoard, and go to the `handson-ml3` directory. Once the server is started, visit *http://localhost:6006/*.

Now you should see TensorBoard's user interface. Click the SCALARS tab to view the learning curves (see Figure 10-16). At the bottom left, select the logs you want to visualize (e.g., the training logs from the first and second run), and click the `epoch_loss` scalar. Notice that the training loss went down nicely during both runs, but the second run went down a bit faster thanks to the higher learning rate.

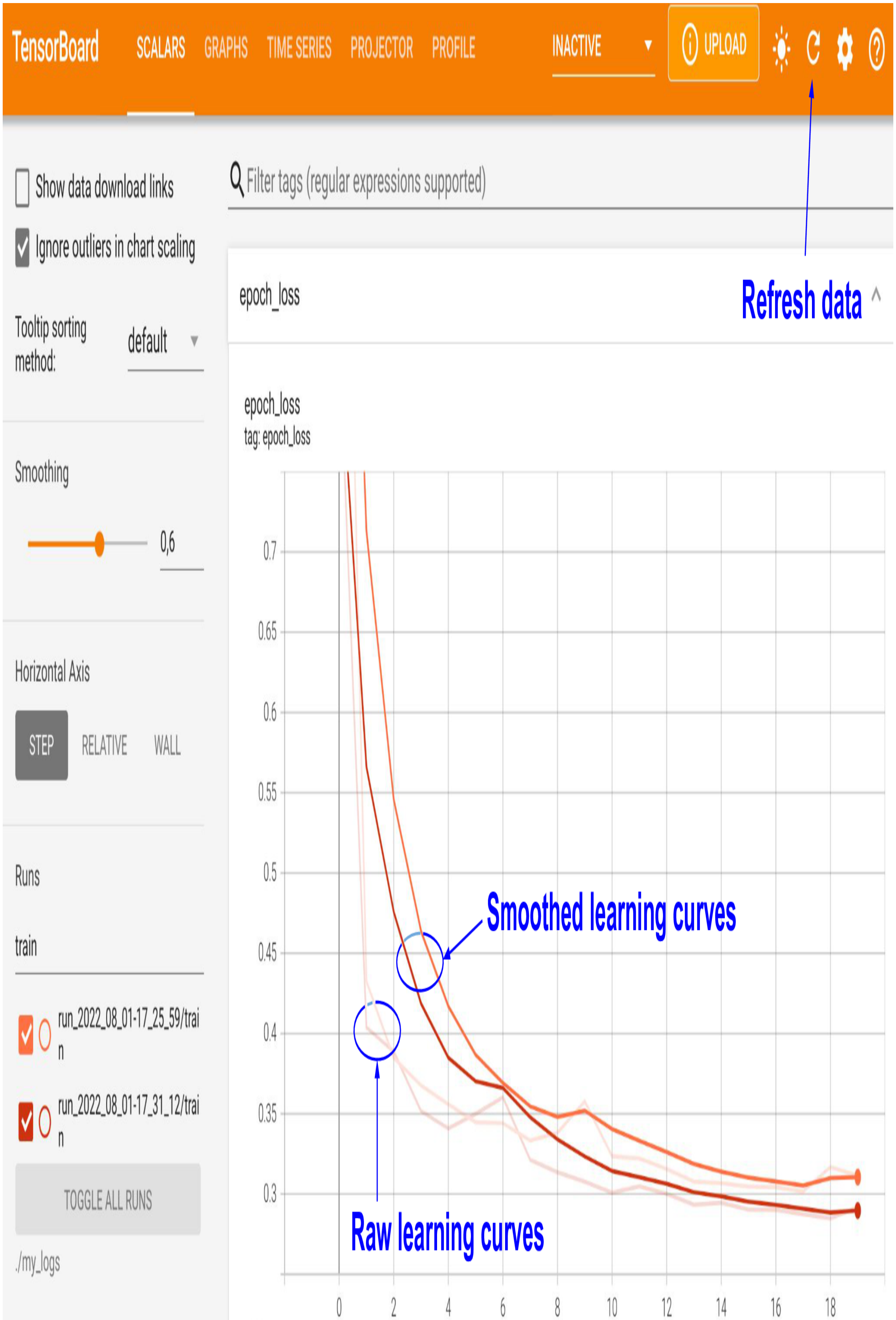

TensorBoard
SCALARS
GRAPHS
TIME SERIES
PROJECTOR
PROFILE
INACTIVE
UPLOAD
Show data download links
Ignore outliers in chart scaling
Tooltip sorting method:
default
Smoothing
0,6
Horizontal Axis
STEP
RELATIVE
WALL
Runs
train
run_2022_08_01-17_25_59/train
run_2022_08_01-17_31_12/train
TOGGLE ALL RUNS
./my_logs
Filter tags (regular expressions supported)
epoch_loss
Refresh data
epoch_loss
tag: epoch_loss
0.7
0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0
2
4
6
8
10
12
14
16
18
Smoothed learning curves
Raw learning curves

Figure 10-16. Visualizing learning curves with TensorBoard

You can also visualize the whole computation graph in the GRAPHS tab, the learned weights projected to 3D in the PROJECTOR tab, and the profiling traces in the PROFILE tab. The `TensorBoard()` callback has options to log extra data too (see the documentation for more details). You can click the refresh button (⟳) at the top right to make TensorBoard refresh data, and you can click the settings button (⚙) to activate auto-refresh and specify the refresh interval.

Additionally, TensorFlow offers a lower-level API in the `tf.summary` package. The following code creates a `SummaryWriter` using the `create_file_writer()` function, and it uses this writer as a Python context to log scalars, histograms, images, audio, and text, all of which can then be visualized using TensorBoard:

```
test_logdir = get_run_logdir()
writer = tf.summary.create_file_writer(str(test_logdir))
with writer.as_default():
    for step in range(1, 1000 + 1):
        tf.summary.scalar("my_scalar", np.sin(step / 10),
step=step)

        data = (np.random.randn(100) + 2) * step / 100  # gets
larger
        tf.summary.histogram("my_hist", data, buckets=50,
step=step)

        images = np.random.rand(2, 32, 32, 3) * step / 1000  #
gets brighter
        tf.summary.image("my_images", images, step=step)

        texts = ["The step is " + str(step), "Its square is " +
str(step ** 2)]
        tf.summary.text("my_text", texts, step=step)

        sine_wave = tf.math.sin(tf.range(12000) / 48000 * 2 *
np.pi * step)
        audio = tf.reshape(tf.cast(sine_wave, tf.float32), [1,
-1, 1])
        tf.summary.audio("my_audio", audio, sample_rate=48000,
step=step)
```

If you run this code and click the refresh button in TensorBoard, you will see several tabs appear: IMAGES, AUDIO, DISTRIBUTIONS, HISTOGRAMS and TEXT. Try clicking on the IMAGES tab, and use the slider above each image to view the images at different time steps. Similarly, go to the AUDIO tab and try listening to the audios at different time steps. As you can see, TensorBoard is a useful tool even beyond TensorFlow or Deep Learning.

> **TIP**
>
> You can share your results online by publishing them to *https://tensorboard.dev*. For this, just run `!tensorboard dev upload --logdir ./my_logs`. The first time, it will ask you to accept the terms and conditions and authenticate. Then your logs will be uploaded, and you will get a permanent link to view your results in a TensorBoard interface.

Let's summarize what you've learned so far in this chapter: you now know where neural nets came from, what an MLP is and how you can use it for classification and regression, how to use Keras's Sequential API to build MLPs, and how to use the Functional API or the Subclassing API to build more complex model architectures, including Wide & Deep models, as well as models with multiple inputs and outputs. You also learned how to save and restore a model and how to use callbacks for checkpointing, early stopping, and more. Finally, you learned how to use TensorBoard for visualization. You can already go ahead and use neural networks to tackle many problems! However, you may wonder how to choose the number of hidden layers, the number of neurons in the network, and all the other hyperparameters. Let's look at this now.

Fine-Tuning Neural Network Hyperparameters

The flexibility of neural networks is also one of their main drawbacks: there are many hyperparameters to tweak. Not only can you use any imaginable network architecture, but even in a basic MLP you can change the number of layers, the number of neurons and the type of activation function to use in each layer, the weight initialization logic, the type of optimizer to use, its learning rate, the batch size, and more. How do you know what combination of hyperparameters is the best for your task?

One option is to convert your Keras model to a Scikit-Learn estimator, and then use `GridSearchCV` or `RandomizedSearchCV` to fine-tune the hyperparameters, as you did in Chapter 2. For this, you can use the `KerasRegressor` and `KerasClassifier` wrapper classes from the SciKeras library (see *https://github.com/adriangb/scikeras* for more details). However, there's a better way: you can use the *Keras Tuner* library, which is a hyperparameter tuning library for Keras models. It offers several tuning strategies, it's highly customizable, and it has excellent integration with TensorBoard. Let's see how to use it.

If you followed the installation instructions at *https://homl.info/install* to run everything locally, then you already have Keras Tuner installed, but if you are using Colab, then you must run `%pip install -q -U keras-tuner`. Next, import `keras_tuner`, usually as `kt`, then write a function that builds, compiles, and returns a Keras model. The function must take a `kt.HyperParameters` object as argument, which it can use to define hyperparameters (integers, floats, strings, etc.) along with their range of possible values, and these hyperparameters may be used to build and compile the model. For example, the following function builds and compiles an MLP to classify Fashion MNIST images, using hyperparameters such as the number of hidden layers (`n_hidden`), the number of neurons per layer (`n_neurons`), the learning rate (`learning_rate`), and the type of optimizer to use (`optimizer`):

```
import keras_tuner as kt

def build_model(hp):
    n_hidden = hp.Int("n_hidden", min_value=0, max_value=8,
default=2)
    n_neurons = hp.Int("n_neurons", min_value=16, max_value=256)
    learning_rate = hp.Float("learning_rate", min_value=1e-4,
```

```
max_value=1e-2,
                                     sampling="log")
    optimizer = hp.Choice("optimizer", values=["sgd", "adam"])
    if optimizer == "sgd":
        optimizer =
tf.keras.optimizers.SGD(learning_rate=learning_rate)
    else:
        optimizer =
tf.keras.optimizers.Adam(learning_rate=learning_rate)

    model = tf.keras.Sequential()
    model.add(tf.keras.layers.Flatten())
    for _ in range(n_hidden):
        model.add(tf.keras.layers.Dense(n_neurons,
activation="relu"))
    model.add(tf.keras.layers.Dense(10, activation="softmax"))
    model.compile(loss="sparse_categorical_crossentropy",
optimizer=optimizer,
                  metrics=["accuracy"])
    return model
```

The first part of the function defines the hyperparameters. For example, `hp.Int("n_hidden", min_value=0, max_value=8, default=2)` checks whether a hyperparameter named `"n_hidden"` is already present in the `HyperParameters` object `hp`, and if so it returns its value. If not, then it registers a new integer hyperparameter named `"n_hidden"`, whose possible values range from 0 to 8 (inclusive), and it returns the default value, which is 2 in this case (when `default` is not set, then `min_value` is returned). The `"n_neurons"` hyperparameter is registered in a similar way. The `"learning_rate"` hyperparameter is registered as a float ranging from 10^{-4} to 10^{-2}, and since `sampling="log"`, learning rates of all scales will be sampled equally. Lastly, the `optimizer` hyperparameter is registered with two possible values: `"sgd"` or `"adam"` (the default value is the first one, which is `"sgd"` in this case). Depending on the value of `optimizer`, we create an `SGD` optimizer or an `Adam` optimizer with the given learning rate.

The second part of the function just builds the model using the hyperparameter values. It creates a `Sequential` model starting with a `Flatten` layer, followed by the requested number of hidden layers (as determined by the `n_hidden` hyperparameter) using the ReLU activation function, and an output layer with 10 neurons (one per class) and using the softmax activation function. Lastly, the function compiles the model and returns it.

Now if you want to do a basic random search, you can create a `kt.RandomSearch` tuner, passing the `build_model` function to the constructor, and call the tuner's `search()` method:

```
random_search_tuner = kt.RandomSearch(
    build_model, objective="val_accuracy", max_trials=5,
overwrite=True,
    directory="my_fashion_mnist", project_name="my_rnd_search",
seed=42)
random_search_tuner.search(X_train, y_train, epochs=10,
                           validation_data=(X_valid, y_valid))
```

The `RandomSearch` tuner first calls `build_model()` once with an empty `Hyperparameters` object, just to gather all the hyperparameters specifications. Then, in this example, it runs 5 trials, and for each trial it builds a model using hyperparameters sampled randomly within their respective ranges, then it trains that model for 10 epochs and saves it to a subdirectory of the `my_fashion_mnist/my_rnd_search` directory. Since `overwrite=True`, the `my_rnd_search` directory is deleted before training starts. If you run this code a second time but with `overwrite=False` and `max_trials=10`, the tuner will continue tuning where it left off, running 5 more trials: this means you don't have to run all the trials in one shot. Lastly, since `objective` is set to `"val_accuracy"`, the tuner prefers models with a higher validation accuracy, so once the tuner has finished searching, you can get the best models like this:

```
top3_models = random_search_tuner.get_best_models(num_models=3)
best_model = top3_models[0]
```

You can also call `get_best_hyperparameters()` to get the `kt.HyperParameters` of the best models:

```
>>> top3_params =
random_search_tuner.get_best_hyperparameters(num_trials=3)
>>> top3_params[0].values  # best hyperparameter values
{'n_hidden': 5,
 'n_neurons': 70,
 'learning_rate': 0.00041268008323824807,
 'optimizer': 'adam'}
```

Each tuner is guided by a so-called *oracle*: before each trial, the tuner asks the oracle to tell it what the next trial should be. The `RandomSearch` tuner uses a `RandomSearchOracle`, which is pretty basic: it just picks the next trial randomly, as we saw earlier. Since the oracle keeps track of all the trials, you can ask it to give you the best one, and you can display a summary of that trial:

```
>>> best_trial =
random_search_tuner.oracle.get_best_trials(num_trials=1)[0]
>>> best_trial.summary()
Trial summary
Hyperparameters:
n_hidden: 5
n_neurons: 70
learning_rate: 0.00041268008323824807
optimizer: adam
Score: 0.8736000061035156
```

This shows the best hyperparameters (like earlier), as well as the validation accuracy. You can also access all the metrics directly:

```
>>> best_trial.metrics.get_last_value("val_accuracy")
0.8736000061035156
```

If you are happy with the best model's performance, you may continue training it for a few epochs on the full training set (`X_train_full` and `y_train_full`), then evaluate it on the test set, and deploy it to production (see Chapter 19):

```
best_model.fit(X_train_full, y_train_full, epochs=10)
test_loss, test_accuracy = best_model.evaluate(X_test, y_test)
```

In some cases, you may want to fine-tune data preprocessing hyperparameters, or `model.fit()` arguments, such as the batch size. For this, you must use a slightly different technique: instead of writing a `build_model()` function, you must subclass the `kt.HyperModel` class and define two methods, `build()` and `fit()`. The `build()` method does the exact same thing as the `build_model()` function, and the `fit()` method takes a `HyperParameters` object and a compiled model as argument, as well as all the `model.fit()` arguments, and it must fit the model and return the `History` object. Crucially, the `fit()` method may use hyperparameters to decide how to preprocess the data, tweak the batch size, and more. For example, the following class builds the same model as before, with the same hyperparameters, but it also uses a boolean `"normalize"` hyperparameter to control whether or not to standardize the training data before fitting the model:

```
class MyClassificationHyperModel(kt.HyperModel):
    def build(self, hp):
        return build_model(hp)

    def fit(self, hp, model, X, y, **kwargs):
        if hp.Boolean("normalize"):
            norm_layer = tf.keras.layers.Normalization()
            X = norm_layer(X)
        return model.fit(X, y, **kwargs)
```

You can then pass an instance of this class to the tuner of your choice, instead of passing the `build_model` function. For example, let’s build a `kt.Hyperband` tuner based on a `MyClassificationHyperModel` instance:

```
hyperband_tuner = kt.Hyperband(
    MyClassificationHyperModel(), objective="val_accuracy",
seed=42,
    max_epochs=10, factor=3, hyperband_iterations=2,
    overwrite=True, directory="my_fashion_mnist",
project_name="hyperband")
```

This tuner is similar to the HalvingRandomSearchCV class we discussed in Chapter 2: it starts by training many different models for few epochs, then it eliminates the worst models and keeps only the top 1 / factor models (i.e., the top third in this case), repeating this selection process until a single model is left.[17] The max_epochs argument controls the max number of epochs that the best model will be trained for. The whole process is repeated twice in this case (hyperband_iterations=2). The total number of training epochs across all models for each hyperband iteration is about max_epochs * (log(max_epochs) / log(factor)) ** 2, so it's about 44 epochs in this example. The other arguments as the same as for kt.RandomSearch.

Let's run the Hyperband tuner now. We'll use the TensorBoard callback, this time pointing to the root log directory (the tuner will take care of using a different subdirectory for each trial), as well as an EarlyStopping callback:

```
root_logdir = Path(hyperband_tuner.project_dir) / "tensorboard"
tensorboard_cb = tf.keras.callbacks.TensorBoard(root_logdir)
early_stopping_cb = tf.keras.callbacks.EarlyStopping(patience=2)
hyperband_tuner.search(X_train, y_train, epochs=10,
                       validation_data=(X_valid, y_valid),
                       callbacks=[early_stopping_cb,
tensorboard_cb])
```

Now if you open TensorBoard, pointing --logdir to the my_fashion_mnist/hyperband/tensorboard directory, you will see all the trial results, as they unfold. Make sure to visit the HPARAMS tab: it contains a summary of all the hyperparameter combinations that were tried, along with the corresponding metrics. Notice that there are three tabs inside the HPARAMS tab: a table view, a parallel coordinates view, and a scatter plot matrix view. In the lower part of the left panel, uncheck all metrics except for validation.epoch_accuracy: this will make the graphs clearer. In the parallel coordinates view, try selecting a range of high values on the validation.epoch_accuracy column: this will filter only the hyperparameter combinations that reached a good performance. Click on one of the hyperparameter combinations: the corresponding learning curves will appear at the bottom of the page. Take some time to go through each tab: they will help you understand the effect of each hyperparameter on performance, as well as the interactions between the hyperparameters.

Hyperband is smarter than pure random search in the way it allocates resources, but at its core it still explores the hyperparameter space randomly: it's fast, but coarse. However, Keras Tuner also includes a `kt.BayesianOptimization` tuner: this algorithm gradually learns which regions of the hyperparameter space are most promising by fitting a probabilistic model called a *Gaussian process*. This allows it to gradually zoom in on the best hyperparameters. The downside is that this algorithm has its own hyperparameters: `alpha` represents the level of noise you expect in the performance measures across trials (it defaults to 10^{-4}), and `beta` specifies how much you want the algorithm to explore, instead of simply exploiting the known good regions of hyperparameter space (it defaults to 2.6). Other than that, this tuner can be used just like the previous ones:

```
bayesian_opt_tuner = kt.BayesianOptimization(
    MyClassificationHyperModel(), objective="val_accuracy",
seed=42,
    max_trials=10, alpha=1e-4, beta=2.6,
    overwrite=True, directory="my_fashion_mnist",
project_name="bayesian_opt")
bayesian_opt_tuner.search([...])
```

Hyperparameter tuning is still an active area of research, and many other approaches are being explored. For example, check out DeepMind's excellent 2017 paper,[18] where the authors used an evolutionary algorithm to jointly optimize a population of models and their hyperparameters. Google has also used an evolutionary approach, not just to search for hyperparameters but also to explore all sorts of model architectures. They offer a hyperparameter tuning service as part of their Google's Vertex AI platform (see Chapter 19). Evolutionary algorithms have even been used successfully to train individual neural networks, replacing the ubiquitous Gradient Descent! For an example, see the 2017 post by Uber where the authors introduce their *Deep Neuroevolution* technique.

But despite all this exciting progress and all these tools and services, it still helps to have an idea of what values are reasonable for each hyperparameter so that you can build a quick prototype and restrict the search space. The following sections provide guidelines for choosing the number of hidden layers and neurons in an MLP and for selecting good values for some of the main hyperparameters.

Number of Hidden Layers

For many problems, you can begin with a single hidden layer and get reasonable results. An MLP with just one hidden layer can theoretically model even the most complex functions, provided it has enough neurons. But for complex problems, deep networks have a much higher *parameter efficiency* than shallow ones: they can model complex functions using exponentially fewer neurons than shallow nets, allowing them to reach much better performance with the same amount of training data.

To understand why, suppose you are asked to draw a forest using some drawing software, but you are forbidden to copy and paste anything. It would take an enormous amount of time: you would have to draw each tree individually, branch by branch, leaf by leaf. If you could instead draw one leaf, copy and paste it to draw a branch, then copy and paste that branch to create a tree, and finally copy and paste this tree to make a forest, you would be finished in no time. Real-world data is often structured in such a hierarchical way, and deep neural networks automatically take advantage of this fact: lower hidden layers model low-level structures (e.g., line segments of various shapes and orientations), intermediate hidden layers combine these low-level structures to model intermediate-level structures (e.g., squares, circles), and the highest hidden layers and the output layer combine these intermediate structures to model high-level structures (e.g., faces).

Not only does this hierarchical architecture help DNNs converge faster to a good solution, but it also improves their ability to generalize to new datasets. For example, if you have already trained a model to recognize faces in pictures and you now want to train a new neural network to recognize hairstyles, you can kickstart the training by reusing the lower layers of the first network. Instead of randomly initializing the weights and biases of the first few layers of the new neural network, you can initialize them to the values of the weights and biases of the lower layers of the first network. This way the network will not have to learn from scratch all the low-level structures that occur in most pictures; it will only have to learn the higher-level structures (e.g., hairstyles). This is called *transfer learning*.

In summary, for many problems you can start with just one or two hidden layers and the neural network will work just fine. For instance, you can easily reach above 97% accuracy on the MNIST dataset using just one hidden layer with a few hundred neurons, and above 98% accuracy using two hidden layers with the same total number of neurons, in roughly the same amount of training time. For more complex problems, you can ramp up the number of hidden layers until you start overfitting the training set. Very complex tasks, such as large image classification or speech recognition, typically require networks with dozens of layers (or even hundreds, but not fully connected ones, as we will see in Chapter 14), and they need a huge amount of training data. You will rarely have to train such networks from scratch: it is much more common to reuse parts of a pretrained state-of-the-art network that performs a similar task. Training will then be a lot faster and require much less data (we will discuss this in Chapter 11).

Number of Neurons per Hidden Layer

The number of neurons in the input and output layers is determined by the type of input and output your task requires. For example, the MNIST task requires 28 × 28 = 784 inputs and 10 output neurons.

As for the hidden layers, it used to be common to size them to form a pyramid, with fewer and fewer neurons at each layer—the rationale being that many low-level features can coalesce into far fewer high-level features. A typical neural network for MNIST might have 3 hidden layers, the first with 300 neurons, the second with 200, and the third with 100. However, this practice has been largely abandoned because it seems that using the same number of neurons in all hidden layers performs just as well in most cases, or even better; plus, there is only one hyperparameter to tune, instead of one per layer. That said, depending on the dataset, it can sometimes help to make the first hidden layer bigger than the others.

Just like the number of layers, you can try increasing the number of neurons gradually until the network starts overfitting. Alternatively, you can try building a model with a bit more layers and neurons than you actually need, then use early stopping and other regularization techniques to prevent it from overfitting too much. Vincent Vanhoucke, a scientist at Google, has dubbed this the "stretch pants" approach: instead of wasting time looking for pants that perfectly match your size, just use large stretch pants that will shrink down to the right size. With this approach, you avoid bottleneck layers that could ruin your model. Indeed, if a layer has too few neurons, it will not have enough representational power to preserve all the useful information from the inputs (e.g., a layer with two neurons can only output 2D data, so if it gets 3D data as input, some information will be lost). No matter how big and powerful the rest of the network is, that information will never be recovered.

> **TIP**
>
> In general you will get more bang for your buck by increasing the number of layers instead of the number of neurons per layer.

Learning Rate, Batch Size, and Other Hyperparameters

The number of hidden layers and neurons are not the only hyperparameters you can tweak in an MLP. Here are some of the most important ones, as well as tips on how to set them:

Learning rate

The learning rate is arguably the most important hyperparameter. In general, the optimal learning rate is about half of the maximum learning rate (i.e., the learning rate above which the training algorithm diverges, as we saw in Chapter 4). One way to find a good learning rate is to train the model for a few hundred iterations, starting with a very low learning rate (e.g., 10^{-5}) and gradually increasing it up to a very large value (e.g., 10). This is done by multiplying the learning rate by a constant factor at each iteration (e.g., by $(10 / 10^{-5})^{1 / 500}$ to go from 10^{-5} to 10 in 500 iterations). If you plot the loss as a function of the learning rate (using a log scale for the learning rate), you should see it dropping at first. But after a while, the learning rate will be too large, so the loss will shoot back up: the optimal learning rate will be a bit lower than the point at which the loss starts to climb (typically about 10 times lower than the turning point). You can then reinitialize your model and train it normally using this good learning rate. We will look at more learning rate techniques in Chapter 11.

Optimizer

Choosing a better optimizer than plain old Mini-batch Gradient Descent (and tuning its hyperparameters) is also quite important. We will see several advanced optimizers in Chapter 11.

Batch size

The batch size can have a significant impact on your model's performance and training time. The main benefit of using large batch sizes is that hardware accelerators like GPUs can process them efficiently (see Chapter 19), so the training algorithm will see more instances per second. Therefore, many researchers and practitioners recommend using the largest batch size that can fit in GPU RAM. There's a catch, though: in practice, large batch sizes often lead to training instabilities, especially at the beginning of training, and the resulting model may not generalize as well as a model trained with a small batch size. In April 2018, Yann LeCun even tweeted “Friends don’t let friends use mini-batches larger than 32,” citing a 2018 paper[19] by Dominic Masters and Carlo Luschi which concluded that using small batches (from 2 to 32) was preferable because small batches led to better models in less training time. Other papers point in the opposite direction, however; in 2017, papers by Elad Hoffer et al.[20] and Priya Goyal et al.[21] showed that it was possible to use very large batch sizes (up to 8,192) using various techniques such as warming up the learning rate (i.e., starting training with a small learning rate, then ramping it up, as we will see in Chapter 11). This led to a very short training time, without any generalization gap. So, one strategy is to try to use a large batch size, using learning rate warmup, and if training is unstable or the final performance is disappointing, then try using a small batch size instead.

Activation function

We discussed how to choose the activation function earlier in this chapter: in general, the ReLU activation function will be a good default for all hidden layers. For the output layer, it really depends on your task.

Number of iterations

In most cases, the number of training iterations does not actually need to be tweaked: just use early stopping instead.

TIP

The optimal learning rate depends on the other hyperparameters—especially the batch size—so if you modify any hyperparameter, make sure to update the learning rate as well.

For more best practices regarding tuning neural network hyperparameters, check out the excellent 2018 paper[22] by Leslie Smith.

This concludes our introduction to artificial neural networks and their implementation with Keras. In the next few chapters, we will discuss techniques to train very deep nets. We will also explore how to customize models using TensorFlow's lower-level API and how to load and preprocess data efficiently using the Data API. And we will dive into other popular neural network architectures: convolutional neural networks for image processing, recurrent neural networks and transformers for sequential data and text, autoencoders for representation learning, and generative adversarial networks to model and generate data.[23]

Exercises

1. The TensorFlow Playground is a handy neural network simulator built by the TensorFlow team. In this exercise, you will train several binary classifiers in just a few clicks, and tweak the model's architecture and its hyperparameters to gain some intuition on how neural networks work and what their hyperparameters do. Take some time to explore the following:

    a. The patterns learned by a neural net. Try training the default neural network by clicking the Run button (top left). Notice how it quickly finds a good solution for the classification task. The neurons in the first hidden layer have learned simple patterns, while the neurons in the second hidden layer have learned to combine the simple patterns of the first hidden layer into more complex patterns. In general, the more layers there are, the more complex the patterns can be.

    b. Activation functions. Try replacing the tanh activation function with a ReLU activation function, and train the network again. Notice that it finds a solution even faster, but this time the boundaries are linear. This is due to the shape of the ReLU function.

c. The risk of local minima. Modify the network architecture to have just one hidden layer with three neurons. Train it multiple times (to reset the network weights, click the Reset button next to the Play button). Notice that the training time varies a lot, and sometimes it even gets stuck in a local minimum.

d. What happens when neural nets are too small. Remove one neuron to keep just two. Notice that the neural network is now incapable of finding a good solution, even if you try multiple times. The model has too few parameters and systematically underfits the training set.

e. What happens when neural nets are large enough. Set the number of neurons to eight, and train the network several times. Notice that it is now consistently fast and never gets stuck. This highlights an important finding in neural network theory: large neural networks rarely get stuck in local minima, and even when they do these local optima are often almost as good as the global optimum. However, they can still get stuck on long plateaus for a long time.

f. The risk of vanishing gradients in deep networks. Select the spiral dataset (the bottom-right dataset under "DATA"), and change the network architecture to have four hidden layers with eight neurons each. Notice that training takes much longer and often gets stuck on plateaus for long periods of time. Also notice that the neurons in the highest layers (on the right) tend to evolve faster than the neurons in the lowest layers (on the left). This problem, called the "vanishing gradients" problem, can be alleviated with better weight initialization and other techniques, better optimizers (such as AdaGrad or Adam), or Batch Normalization (discussed in Chapter 11).

g. Go further. Take an hour or so to play around with other parameters and get a feel for what they do, to build an intuitive understanding about neural networks.

2. Draw an ANN using the original artificial neurons (like the ones in Figure 10-3) that computes $A \oplus B$ (where $\oplus$ represents the XOR operation). Hint: $A \oplus B = (A \wedge \neg B) \vee (\neg A \wedge B)$.

3. Why is it generally preferable to use a Logistic Regression classifier rather than a classical Perceptron (i.e., a single layer of threshold logic units trained using the Perceptron training algorithm)? How can you tweak a Perceptron to make it equivalent to a Logistic Regression classifier?

4. Why was the sigmoid activation function a key ingredient in training the first MLPs?

5. Name three popular activation functions. Can you draw them?

6. Suppose you have an MLP composed of one input layer with 10 passthrough neurons, followed by one hidden layer with 50 artificial neurons, and finally one output layer with 3 artificial neurons. All artificial neurons use the ReLU activation function.

   - What is the shape of the input matrix $\mathbf{X}$?
   - What are the shapes of the hidden layer's weight matrix $\mathbf{W}_h$ and bias vector $\mathbf{b}_h$?
   - What are the shapes of the output layer's weight matrix $\mathbf{W}_o$ and bias vector $\mathbf{b}_o$?
   - What is the shape of the network's output matrix $\mathbf{Y}$?
   - Write the equation that computes the network's output matrix $\mathbf{Y}$ as a function of $\mathbf{X}$, $\mathbf{W}_h$, $\mathbf{b}_h$, $\mathbf{W}_o$, and $\mathbf{b}_o$.

7. How many neurons do you need in the output layer if you want to classify email into spam or ham? What activation function should

you use in the output layer? If instead you want to tackle MNIST, how many neurons do you need in the output layer, and which activation function should you use? What about for getting your network to predict housing prices, as in Chapter 2?

8. What is backpropagation and how does it work? What is the difference between backpropagation and reverse-mode autodiff?

9. Can you list all the hyperparameters you can tweak in a basic MLP? If the MLP overfits the training data, how could you tweak these hyperparameters to try to solve the problem?

10. Train a deep MLP on the MNIST dataset (you can load it using `tf.keras.datasets.mnist.load_data()`. See if you can get over 98% accuracy by manually tuning the hyperparameters. Try searching for the optimal learning rate by using the approach presented in this chapter (i.e., by growing the learning rate exponentially, plotting the loss, and finding the point where the loss shoots up). Next, try tuning the hyperparameters using Keras Tuner with all the bells and whistles—save checkpoints, use early stopping, and plot learning curves using TensorBoard.

Solutions to these exercises are available at the end of this chapter's notebook, at *https://homl.info/colab3*.

---

1 You can get the best of both worlds by being open to biological inspirations without being afraid to create biologically unrealistic models, as long as they work well.

2 Warren S. McCulloch and Walter Pitts, "A Logical Calculus of the Ideas Immanent in Nervous Activity," *The Bulletin of Mathematical Biology* 5, no. 4 (1943): 115–113.

3 They are not actually attached, just so close that they can very quickly exchange chemical signals.

4 Image by Bruce Blaus (Creative Commons 3.0). Reproduced from *https://en.wikipedia.org/wiki/Neuron*.

5 In the context of Machine Learning, the phrase "neural networks" generally refers to ANNs, not BNNs.

6 Drawing of a cortical lamination by S. Ramon y Cajal (public domain). Reproduced from *https://en.wikipedia.org/wiki/Cerebral_cortex*.

7 Note that this solution is not unique: when data points are linearly separable, there is an infinity of hyperplanes that can separate them.

8 For example, when the inputs are (0, 1), the lower left neuron computes 0×1 + 1×1 – 3/2 = –1/2, which is negative so it outputs 0. The lower right neuron computes 0×1 + 1×1 – 1/2 = 1/2 which is positive so it outputs 1. The output neuron receives the outputs of the first two neurons as its inputs, so it computes 0×(–1) + 1×1 - 1/2 = 1/2, which is positive so it outputs 1.

9 In the 1990s, an ANN with more than two hidden layers was considered deep. Nowadays, it is common to see ANNs with dozens of layers, or even hundreds, so the definition of "deep" is quite fuzzy.

10 David Rumelhart et al. "Learning Internal Representations by Error Propagation," (Defense Technical Information Center technical report, September 1985).

11 Biological neurons seem to implement a roughly sigmoid (*S*-shaped) activation function, so researchers stuck to sigmoid functions for a very long time. But it turns out that ReLU generally works better in ANNs. This is one of the cases where the biological analogy was perhaps misleading.

12 Project ONEIROS (Open-ended Neuro-Electronic Intelligent Robot Operating System).

13 You can also use `tf.keras.utils.plot_model()` to generate an image of your model.

14 Heng-Tze Cheng et al., "Wide & Deep Learning for Recommender Systems," *Proceedings of the First Workshop on Deep Learning for Recommender Systems* (2016): 7–10.

15 The short path can also be used to provide manually engineered features to the neural network.

16 Keras models have an `output` attribute, so we cannot use that name for the main output layer, which is why we renamed it to `main_output`.

17 Hyperband is actually a bit more sophisticated than successive halving, see the paper by Lisha Li et al., "Hyperband: A Novel Bandit-Based Approach to Hyperparameter Optimization," *Journal of Machine Learning Research* 18 (April 2018): 1–52.

18 Max Jaderberg et al., "Population Based Training of Neural Networks," arXiv preprint arXiv:1711.09846 (2017).

19 Dominic Masters and Carlo Luschi, "Revisiting Small Batch Training for Deep Neural Networks," arXiv preprint arXiv:1804.07612 (2018).

20 Elad Hoffer et al., "Train Longer, Generalize Better: Closing the Generalization Gap in Large Batch Training of Neural Networks," *Proceedings of the 31st International Conference on Neural Information Processing Systems* (2017): 1729–1739.

21 Priya Goyal et al., "Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour," arXiv preprint arXiv:1706.02677 (2017).

22 Leslie N. Smith, “A Disciplined Approach to Neural Network Hyper-Parameters: Part 1—Learning Rate, Batch Size, Momentum, and Weight Decay,” arXiv preprint arXiv:1803.09820 (2018).

23 A few extra ANN architectures are presented in the online notebook at *https://homl.info/extra-anns*.

Chapter 11. Training Deep Neural Networks

A NOTE FOR EARLY RELEASE READERS

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.

This will be the 11th chapter of the final book. Notebooks are available on GitHub at *https://github.com/ageron/handson-ml3*. Datasets are available at *https://github.com/ageron/data*.

If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the editoor at ntache@oreilly.com.

In Chapter 10 you built, trained, and fine-tuned your first artificial neural networks. But they were shallow nets, with just a few hidden layers. What if you need to tackle a complex problem, such as detecting hundreds of types of objects in high-resolution images? You may need to train a much deeper ANN, perhaps with 10 layers or many more, each containing hundreds of neurons, linked by hundreds of thousands of connections. Training a deep neural network isn't a walk in the park. Here are some of the problems you could run into:

- You may be faced with the tricky *vanishing gradients* problem or the related *exploding gradients* problem. This is when the gradients grow smaller and smaller, or larger and larger, when flowing backward through the DNN during training. Both of these problems make lower layers very hard to train.

- You might not have enough training data for such a large network, or it might be too costly to label.
- Training may be extremely slow.
- A model with millions of parameters would severely risk overfitting the training set, especially if there are not enough training instances or if they are too noisy.

In this chapter we will go through each of these problems and present techniques to solve them. We will start by exploring the vanishing and exploding gradients problems and some of their most popular solutions. Next, we will look at transfer learning and unsupervised pretraining, which can help you tackle complex tasks even when you have little labeled data. Then we will discuss various optimizers that can speed up training large models tremendously. Finally, we will go through a few popular regularization techniques for large neural networks.

With these tools, you will be able to train very deep nets. Welcome to Deep Learning!

The Vanishing/Exploding Gradients Problems

As we discussed in Chapter 10, the backpropagation algorithm's second phase works by going from the output layer to the input layer, propagating the error gradient along the way. Once the algorithm has computed the gradient of the cost function with regard to each parameter in the network, it uses these gradients to update each parameter with a Gradient Descent step.

Unfortunately, gradients often get smaller and smaller as the algorithm progresses down to the lower layers. As a result, the Gradient Descent update leaves the lower layers' connection weights virtually unchanged, and training never converges to a good solution. This is called the *vanishing gradients* problem. In some cases, the opposite can happen: the gradients can grow bigger and bigger until layers get insanely large weight updates and the algorithm diverges. This is the *exploding gradients* problem, which surfaces most often in recurrent neural networks (see Chapter 16). More generally, deep neural networks suffer from unstable gradients; different layers may learn at widely different speeds.

This unfortunate behavior was empirically observed long ago, and it was one of the reasons deep neural networks were mostly abandoned in the early 2000s. It wasn't clear what caused the gradients to be so unstable when training a DNN, but some light was shed in a 2010 paper by Xavier Glorot and Yoshua Bengio.[1] The authors found a few suspects, including the combination of the popular sigmoid (logistic) activation function and the weight initialization technique that was most popular at the time (i.e., a normal distribution with a mean of 0 and a standard deviation of 1). In short, they showed that with this activation function and this initialization scheme, the variance of the outputs of each layer is much greater than the variance of its inputs. Going forward in the network, the variance keeps increasing after each layer until the activation function saturates at the top layers. This saturation is actually made worse by the fact that the sigmoid function has a mean of 0.5, not 0 (the hyperbolic tangent function has a mean of 0 and behaves slightly better than the sigmoid function in deep networks).

Looking at the sigmoid activation function (see Figure 11-1), you can see that when inputs become large (negative or positive), the function saturates at 0 or 1, with a derivative extremely close to 0 (i.e., the curve is flat at both extremes). Thus, when backpropagation kicks in it has virtually no gradient to propagate back through the network; and what little gradient exists keeps getting diluted as backpropagation progresses down through the top layers, so there is really nothing left for the lower layers.

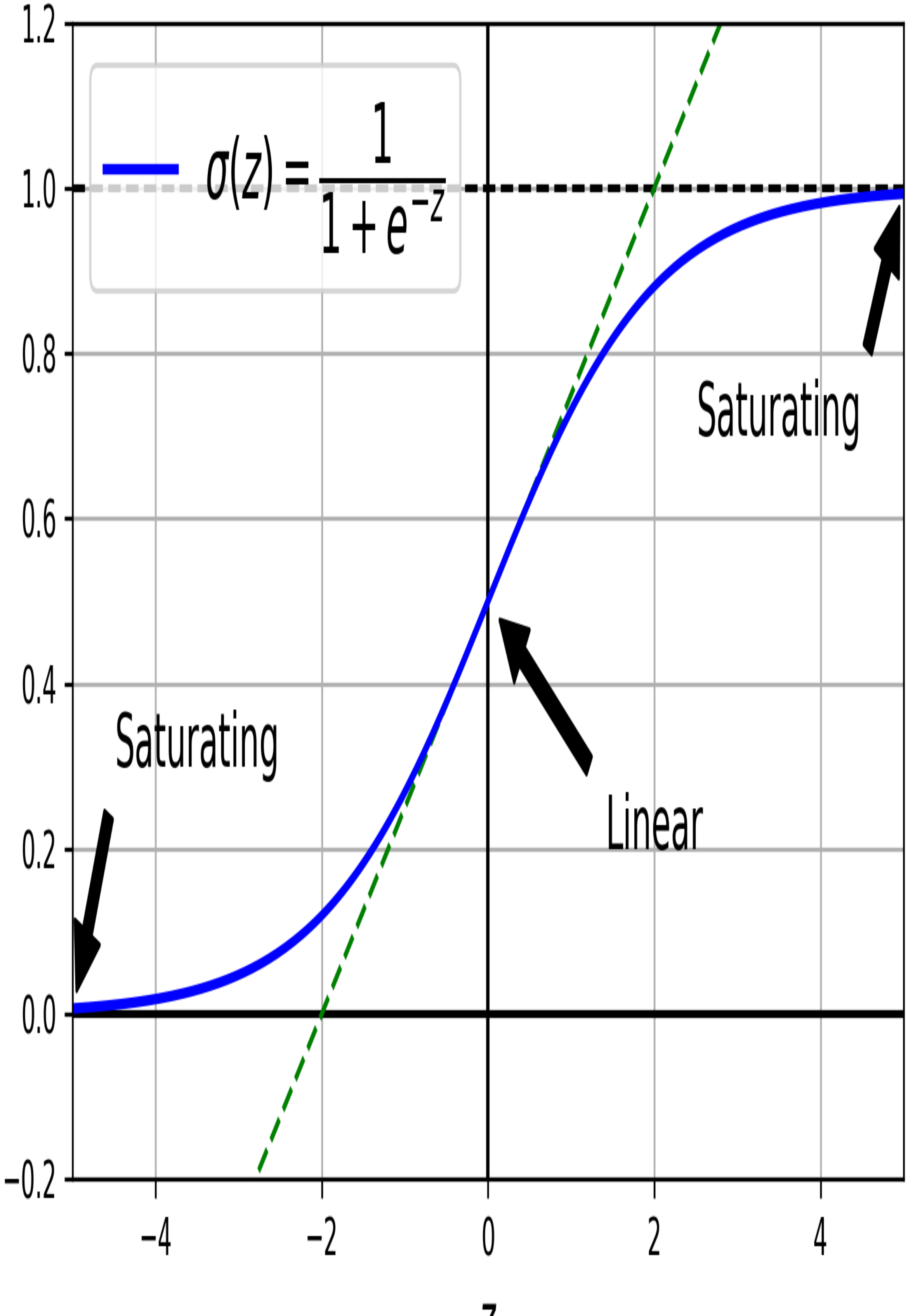

$\sigma(z) = \frac{1}{1 + e^{-z}}$
Saturating
Linear
Saturating
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−4
−2
0
2
4
z

Figure 11-1. Sigmoid activation function saturation

Glorot and He Initialization

In their paper, Glorot and Bengio propose a way to significantly alleviate the unstable gradients problem. They point out that we need the signal to flow properly in both directions: in the forward direction when making predictions, and in the reverse direction when backpropagating gradients. We don't want the signal to die out, nor do we want it to explode and saturate. For the signal to flow properly, the authors argue that we need the variance of the outputs of each layer to be equal to the variance of its inputs,[2] and we need the gradients to have equal variance before and after flowing through a layer in the reverse direction (please check out the paper if you are interested in the mathematical details). It is actually not possible to guarantee both unless the layer has an equal number of inputs and outputs (these numbers are called the *fan-in* and *fan-out* of the layer), but Glorot and Bengio proposed a good compromise that has proven to work very well in practice: the connection weights of each layer must be initialized randomly as described in Equation 11-1, where $fan_{\text{avg}} = (fan_{\text{in}} + fan_{\text{out}})/2$. This initialization strategy is called *Xavier initialization* or *Glorot initialization*, after the paper's first author.

Equation 11-1. Glorot initialization (when using the sigmoid activation function)

$$\text{Normal distribution with mean 0 and variance } \sigma^2 = \frac{1}{fan_{\text{avg}}}$$

$$\text{Or a uniform distribution between } -r \text{ and } +r\text{, with } r = \sqrt{\frac{3}{fan_{\text{avg}}}}$$

If you replace fan_{avg} with fan_{in} in Equation 11-1, you get an initialization strategy that Yann LeCun proposed in the 1990s. He called it *LeCun initialization*. Genevieve Orr and Klaus-Robert Müller even recommended it in their 1998 book *Neural Networks: Tricks of the Trade* (Springer). LeCun initialization is equivalent to Glorot initialization when $fan_{\text{in}} = fan_{\text{out}}$. It took over a decade for researchers to realize how important this trick is. Using Glorot initialization can speed up training considerably, and it is one of the tricks that led to the success of Deep Learning.

Some papers[3] have provided similar strategies for different activation functions. These strategies differ only by the scale of the variance and whether they use fan_{avg} or fan_{in}, as shown in Table 11-1 (for the uniform distribution, just use $r = \sqrt{3\sigma^2}$). The initialization strategy for the ReLU activation function and its variants is called *He initialization* or *Kaiming initialization*, after the paper's first author. For SELU, use Yann LeCun's initialization method, preferably with a Normal distribution. We will cover all these activation functions shortly.

Table 11-1. Initialization paramete

rsforeach type of activation function

Initialization	Activation functions	σ^2 (Normal)
Xavier Glorot	None, tanh, sigmoid, softmax	$1 / fan_{avg}$
Kaiming He	ReLU, Leaky ReLU, ELU, GELU, Swish, Mish	$2 / fan_{in}$
Yann LeCun	SELU	$1 / fan_{in}$

By default, Keras uses Glorot initialization with a uniform distribution. When creating a layer, you can change this to He initialization by setting `kernel_initializer="he_uniform"` or `kernel_initializer="he_normal"` like this:

```
import tensorflow as tf

dense = tf.keras.layers.Dense(50, activation="relu",
                              kernel_initializer="he_normal")
```

Alternatively, you can obtain any of the initializations listed in Table 11-1 and more using the `VarianceScaling` initializer. For example, if you want He initialization with a uniform distribution and based on fan_{avg} (rather than fan_{in}), you can use the following code:

```
he_avg_init = tf.keras.initializers.VarianceScaling(scale=2.,
mode="fan_avg",

distribution="uniform")
dense = tf.keras.layers.Dense(50, activation="sigmoid",
                              kernel_initializer=he_avg_init)
```

Better Activation Functions

One of the insights in the 2010 paper by Glorot and Bengio was that the problems with unstable gradients were in part due to a poor choice of activation function. Until then most people had assumed that if Mother

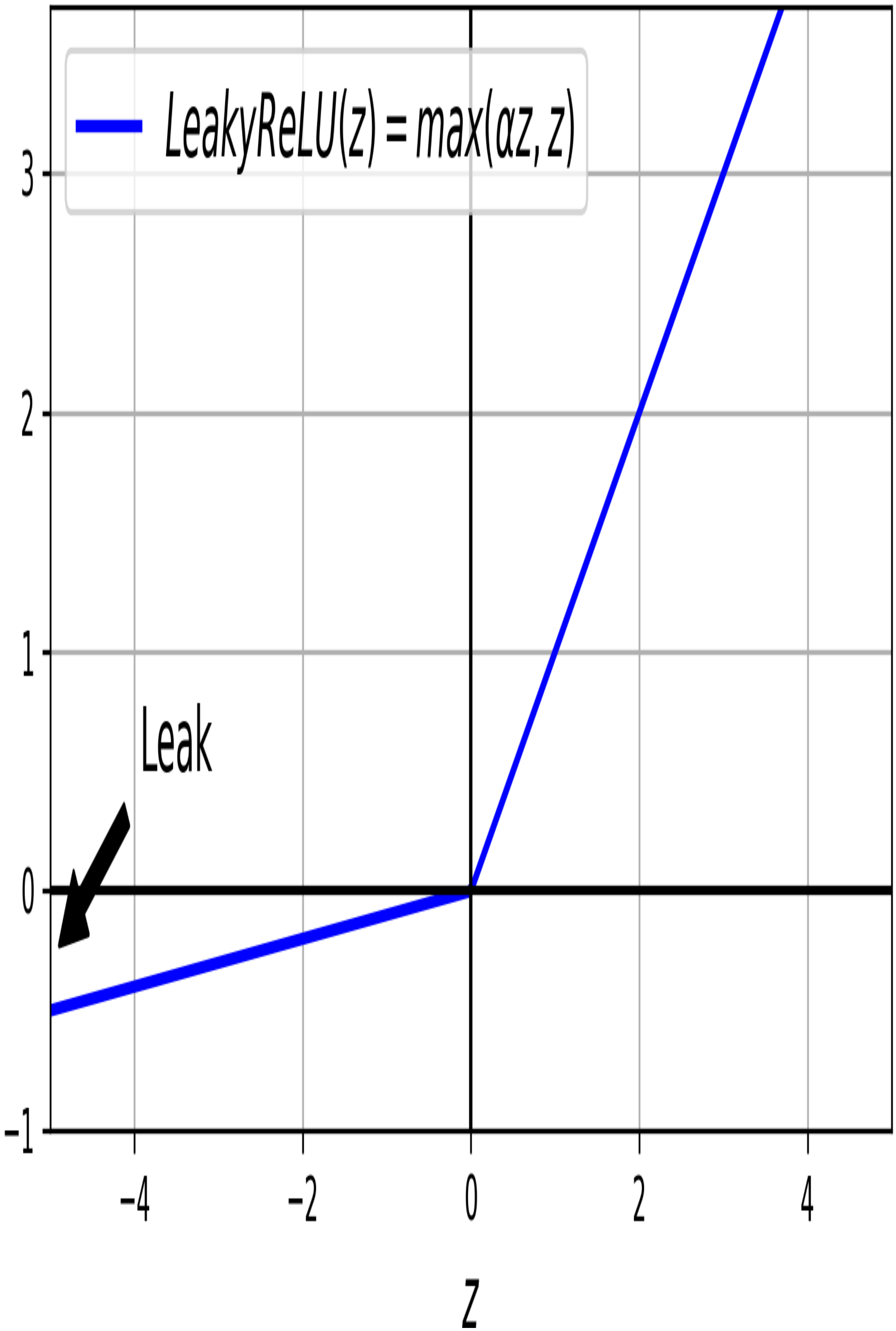
Nature had chosen to use roughly sigmoid activation functions in biological neurons, they must be an excellent choice. But it turns out that other activation functions behave much better in deep neural networks—in particular, the ReLU activation function, mostly because it does not saturate for positive values, and also because it is very fast to compute.

Unfortunately, the ReLU activation function is not perfect. It suffers from a problem known as the *dying ReLUs*: during training, some neurons effectively "die," meaning they stop outputting anything other than 0. In some cases, you may find that half of your network's neurons are dead, especially if you used a large learning rate. A neuron dies when its weights get tweaked in such a way that the input of the ReLU function (i.e., the weighted sum of the neuron's inputs plus its bias term) is negative for all instances in the training set. When this happens, it just keeps outputting zeros, and Gradient Descent does not affect it anymore because the gradient of the ReLU function is zero when its input is negative.[4]

To solve this problem, you may want to use a variant of the ReLU function, such as the *leaky ReLU*.

Leaky ReLU

The leaky ReLU activation function is defined as $\text{LeakyReLU}_{\alpha}(z) = \max(\alpha z, z)$ (see Figure 11-2). The hyperparameter α defines how much the function "leaks": it is the slope of the function for $z < 0$. Having a slope for $z < 0$ ensures that leaky ReLUs never die; they can go into a long coma, but they have a chance to eventually wake up. A 2015 paper by Bing Xu et al.[5] compared several variants of the ReLU activation function, and one of its conclusions was that the leaky variants always outperformed the strict ReLU activation function. In fact, setting $\alpha = 0.2$ (a huge leak) seemed to result in better performance than $\alpha = 0.01$ (a small leak). The paper also evaluated the *randomized leaky ReLU* (RReLU), where α is picked randomly in a given range during training and is fixed to an average value during testing. RReLU also performed fairly well and seemed to act as a regularizer, reducing the risk of overfitting the training set. Finally, the paper evaluated the *parametric leaky ReLU* (PReLU), where α is authorized to be learned during training: instead of being a hyperparameter, it becomes a parameter that can be modified by backpropagation like any other parameter. PReLU was reported to strongly outperform ReLU on large image datasets, but on smaller datasets it runs the risk of overfitting the training set.



$LeakyReLU(z) = max(\alpha z, z)$
Leak
3
2
1
0
−1
−4
−2
0
2
4
z

Figure 11-2. Leaky ReLU: like ReLU, but with a small slope for negative values

Keras includes the classes `LeakyReLU` and `PReLU` in the `tf.keras.layers` package. Just like for other ReLU variants, you should use He initialization, for example:

```
leaky_relu = tf.keras.layers.LeakyReLU(alpha=0.2)  # defaults to
alpha=0.3
dense = tf.keras.layers.Dense(50, activation=leaky_relu,
                              kernel_initializer="he_normal")
```

If you prefer, you can also use `LeakyReLU` as a separate layer in your model, it makes no difference for training and predictions:

```
model = tf.keras.models.Sequential([
    [...]  # more layers
    tf.keras.layers.Dense(50, kernel_initializer="he_normal"),  #
no activation
    tf.keras.layers.LeakyReLU(alpha=0.2),  # activation as a
separate layer
    [...]  # more layers
])
```

For PReLU, replace `LeakyReLU` with `PReLU`. There is currently no official implementation of RReLU in Keras, but you can fairly easily implement your own (to learn how to do that, see the exercises at the end of Chapter 12).

ReLU, leaky ReLU, and PReLU all suffer from the fact that they are not smooth functions: their derivatives abruptly change (at $z = 0$). As we saw in Chapter 4 when we discussed Lasso, this sort of discontinuity can make Gradient Descent bounce around the optimum, and slow down convergence. So now we will look at smooth variants of the ReLU activation function, starting with ELU and SELU.

ELU and SELU

In a 2016 paper by Djork-Arné Clevert et al.[6] proposed a new activation function called the *exponential linear unit* (ELU) that outperformed all the

ReLU variants in the authors' experiments: training time was reduced, and the neural network performed better on the test set. Equation 11-2 shows this activation function's definition.

Equation 11-2. ELU activation function

$$\mathrm{ELU}_\alpha\left(z\right) = \begin{cases} \alpha(\exp\left(z\right) - 1) & \text{if } z < 0 \\ z & \text{if } z \geq 0 \end{cases}$$

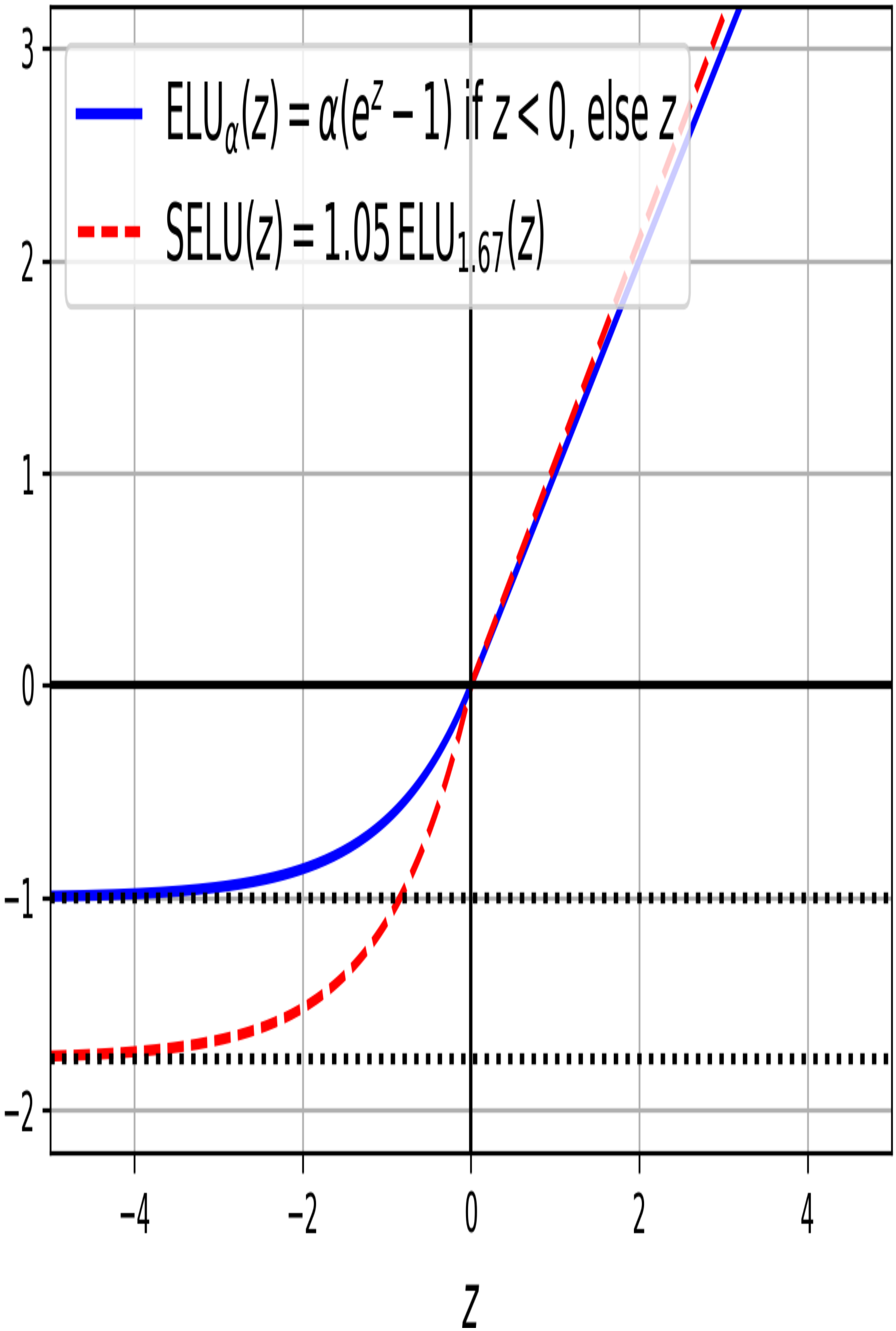
The ELU activation function looks a lot like the ReLU function (see Figure 11-3), with a few major differences:

- It takes on negative values when $z < 0$, which allows the unit to have an average output closer to 0 and helps alleviate the vanishing gradients problem. The hyperparameter α defines the opposite of the value that the ELU function approaches when z is a large negative number. It is usually set to 1, but you can tweak it like any other hyperparameter.

- It has a nonzero gradient for $z < 0$, which avoids the dead neurons problem.

- If α is equal to 1 then the function is smooth everywhere, including around $z = 0$, which helps speed up Gradient Descent since it does not bounce as much to the left and right of $z = 0$.

Using ELU with Keras is as easy as setting `activation="elu"`, and like with other ReLU variants, you should use He initialization. The main drawback of the ELU activation function is that it is slower to compute than the ReLU function and its variants (due to the use of the exponential function). Its faster convergence rate during training may compensate for that slow computation, but still, at test time an ELU network will be a bit slower than a ReLU network.



$\mathrm{ELU}_\alpha(z) = \alpha(e^z - 1)$ if $z < 0$, else z
$\mathrm{SELU}(z) = 1.05\,\mathrm{ELU}_{1.67}(z)$
3
2
1
0
−1
−2
−4
−2
0
2
4
z

Figure 11-3. ELU and SELU activation functions

A year after ELU, a 2017 paper by Günter Klambauer et al.[7] introduced the Scaled ELU (SELU) activation function: as its name suggests, it is a scaled variant of the ELU activation function (about 1.05 times ELU, using $\alpha \approx 1.67$). The authors showed that if you build a neural network composed exclusively of a stack of dense layers (i.e., an MLP), and if all hidden layers use the SELU activation function, then the network will *self-normalize*: the output of each layer will tend to preserve a mean of 0 and a standard deviation of 1 during training, which solves the vanishing/exploding gradients problem. As a result, the SELU activation function may outperform other activation functions for MLPs, especially deep ones. To use it with Keras, just set `activation="selu"`. There are, however, a few conditions for self-normalization to happen (see the paper for the mathematical justification):

- The input features must be standardized: mean 0 and standard deviation 1.
- Every hidden layer's weights must be initialized using LeCun normal initialization. In Keras, this means setting `kernel_initializer="lecun_normal"`.
- The self-normalizing property is only guaranteed with plain MLPs. If you try to use SELU in other architectures, like recurrent networks (see Chapter 16) or networks with *skip connections* (i.e., connections that skip layers, such as in Wide & Deep nets), it will probably not outperform ELU.
- You cannot use regularization techniques like ℓ_1 or ℓ_2 regularization, max-norm, batch-norm or regular dropout (these are discussed later in this chapter).

These are significant constraints, so despite its promises, SELU did not gain a lot of traction. Moreover, three more activation functions seem to outperform it quite consistently on most tasks: GELU, Swish and Mish.

GELU, Swish and Mish

GELU was introduced in a 2016 paper by Dan Hendrycks and Kevin Gimpel.[8] Once again, you can think of it as a smooth variant of the ReLU activation function. Its definition is given in Equation 11-3, where Φ is the standard Gaussian cumulative distribution function (CDF): $\Phi(z)$ corresponds to the probability that a value sampled randomly from a Normal distribution of mean 0 and variance 1 is lower than z.

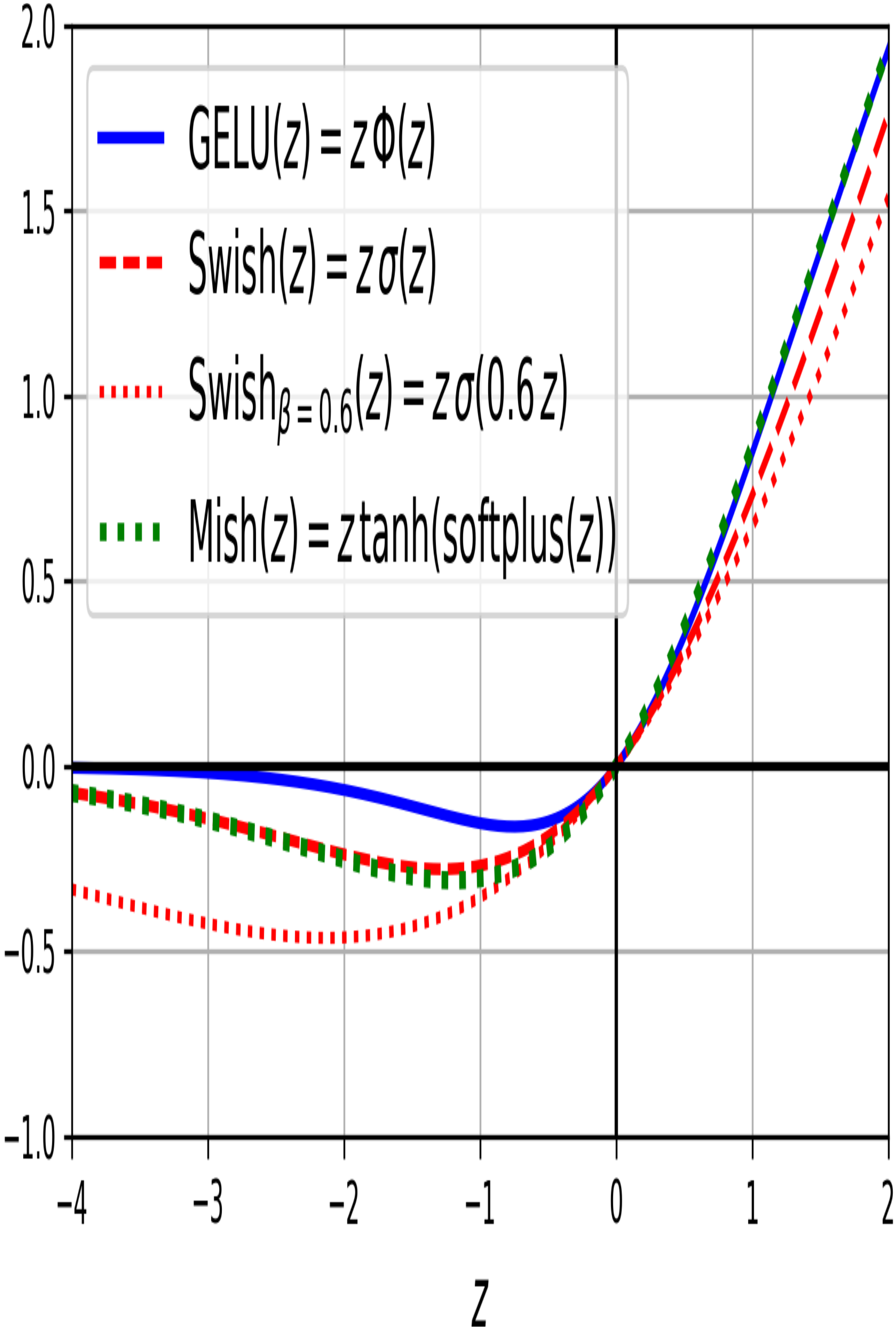
Equation 11-3. GELU activation function

$$\mathrm{GELU}(z) = z\,\Phi(z)$$

As you can see in Figure 11-4, GELU resembles ReLU: it approaches 0 when its input z is very negative, and it approaches z when z is very positive. However, whereas all activation functions we discussed so far were both convex and monotonic,[9] the GELU activation function is neither: from left to right, it starts by going straight, then it wiggles down, reaches a low point around $z \approx -0.75$, and finally it bounces up and ends up going straight towards the top-right. This fairly complex shape and the fact that it has a curvature at every point may explain why it works so well, especially for complex tasks: Gradient Descent may find it easier to fit complex patterns. In practice, it often outperforms every other activation function discussed so far. However, it is a bit more computationally intensive, and the performance boost it provides is not always sufficient to justify the extra cost. That said, it is possible to show that it is approximately equal to $z\sigma(1.702\,z)$, where σ is the sigmoid function: using this approximation also works very well, and it has the advantage of being much faster to compute. In fact, the GELU paper also introduced the SiLU activation function, which is equal to $z\sigma(z)$, but it was outperformed by GELU in their tests.

Interestingly, a 2017 paper by Prajit Ramachandran et al. rediscovered the SiLU function by automatically searching for good activation functions.[10] They named it *Swish*, and the name caught on. In their paper, Swish outperformed every other function, including GELU. The authors later generalized Swish by adding an extra hyperparameter β to scale the sigmoid function's input. The generalized Swish function is $\text{Swish}_\beta(z) = z\sigma(\beta z)$, so GELU is approximately equal to the generalized Swish function using β = 1.702. You can tune β like any other hyperparameter. Alternatively, it's also possible to make β trainable and let Gradient Descent optimize it: much like PReLU, this can make your model more powerful, but it also runs the risk of overfitting the data.

Another quite similar activation function is *Mish*, which was introduced in a 2019 paper by Diganta Misra.[11] It is defined as $\text{mish}(z) = z\tanh(\text{softplus}(z))$, where $\text{softplus}(z) = \log(1 + \exp(z))$. Just like GELU and Swish, it is a smooth, non-convex, and non-monotonic variant of ReLU, and once again the author ran many experiments and found that Mish generally outperformed other activation functions, even Swish and GELU by a tiny margin. Figure 11-4 shows GELU, Swish (both with the default $\beta = 1$ and with $\beta = 0.6$), and lastly Mish. As you can see, Mish overlaps almost perfectly with Swish when z is negative, and almost perfectly with GELU when z is positive.



GELU(z) = zΦ(z)
Swish(z) = zσ(z)
Swish_{β = 0.6}(z) = zσ(0.6 z)
Mish(z) = z tanh(softplus(z))
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−4
−3
−2
−1
0
1
2
z

Figure 11-4. GELU, Swish, parametrized Swish, and Mish activation functions

Keras supports GELU and Swish out of the box, just use `activation="gelu"` or `activation="swish"`. However, it does not support Mish or the generalized Swish activation function yet (but see Chapter 12 to see how to implement your own activation functions and layers).

> **TIP**
>
> So, which activation function should you use for the hidden layers of your deep neural networks? ReLU remains a good default for simple tasks: it's often just as good as the more sophisticated activation functions, plus it's very fast to compute, and many libraries and hardware accelerators provide ReLU-specific optimizations. However, Swish is probably a better default for more complex tasks, and you can even try parametrized Swish with a learnable β parameter for the most complex tasks. Mish may give you very slightly better results, but it requires a bit more compute. If you care a lot about runtime latency, then you may prefer leaky ReLU, or parametrized leaky ReLU for more complex tasks. For deep MLPs, give SELU a try, but make sure to respect the constraints listed earlier. If you have spare time and computing power, you can use cross-validation to evaluate other activation functions as well.

That's all for activation functions! Now, let's look at a completely different way to solve the unstable gradients problem: Batch Normalization.

Batch Normalization

Although using He initialization along with ReLU (or any of its variants) can significantly reduce the danger of the vanishing/exploding gradients problems at the beginning of training, it doesn't guarantee that they won't come back during training.

In a 2015 paper,[12] Sergey Ioffe and Christian Szegedy proposed a technique called *Batch Normalization* (BN) that addresses these problems. The technique consists of adding an operation in the model just before or after the activation function of each hidden layer. This operation simply zero-centers and normalizes each input, then scales and shifts the result using two new parameter vectors per layer: one for scaling, the other for shifting. In other words, the operation lets the model learn the optimal scale and mean of each of the layer's inputs. In many cases, if you add a BN layer as the very first layer of your neural network, you do not need to standardize your training set (i.e., no need for `StandardScaler` or `Normalization`); the BN layer will do it for you (well, approximately, since it only looks at one batch at a time, and it can also rescale and shift each input feature).

In order to zero-center and normalize the inputs, the algorithm needs to estimate each input's mean and standard deviation. It does so by evaluating the mean and standard deviation of the input over the current mini-batch (hence the name "Batch Normalization"). The whole operation is summarized step by step in Equation 11-4.

Equation 11-4. Batch Normalization algorithm

$$
\begin{aligned}
&1. \quad \boldsymbol{\mu}_B = \frac{1}{m_B} \sum_{i=1}^{m_B} \mathbf{x}^{(i)} \\
&2. \quad {\boldsymbol{\sigma}_B}^2 = \frac{1}{m_B} \sum_{i=1}^{m_B} \left(\mathbf{x}^{(i)} - \boldsymbol{\mu}_B\right)^2 \\
&3. \quad \widehat{\mathbf{x}}^{(i)} = \frac{\mathbf{x}^{(i)} - \boldsymbol{\mu}_B}{\sqrt{{\boldsymbol{\sigma}_B}^2 + \varepsilon}} \\
&4. \quad \mathbf{z}^{(i)} = \boldsymbol{\gamma} \otimes \widehat{\mathbf{x}}^{(i)} + \boldsymbol{\beta}
\end{aligned}
$$

In this algorithm:

- $\boldsymbol{\mu}_B$ is the vector of input means, evaluated over the whole mini-batch B (it contains one mean per input).
- m_B is the number of instances in the mini-batch.
- $\boldsymbol{\sigma}_B$ is the vector of input standard deviations, also evaluated over the whole mini-batch (it contains one standard deviation per input).

- $\hat{\mathbf{x}}^{(i)}$ is the vector of zero-centered and normalized inputs for instance i.

- ε is a tiny number that avoids division by zero and ensures the gradients don't grow too large (typically 10^{-5}). This is called a *smoothing term*.

- $\boldsymbol{\gamma}$ is the output scale parameter vector for the layer (it contains one scale parameter per input).

- $\otimes$ represents element-wise multiplication (each input is multiplied by its corresponding output scale parameter).

- $\boldsymbol{\beta}$ is the output shift (offset) parameter vector for the layer (it contains one offset parameter per input). Each input is offset by its corresponding shift parameter.

- $\mathbf{z}^{(i)}$ is the output of the BN operation. It is a rescaled and shifted version of the inputs.

So during training, BN standardizes its inputs, then rescales and offsets them. Good! What about at test time? Well, it's not that simple. Indeed, we may need to make predictions for individual instances rather than for batches of instances: in this case, we will have no way to compute each input's mean and standard deviation. Moreover, even if we do have a batch of instances, it may be too small, or the instances may not be independent and identically distributed, so computing statistics over the batch instances would be unreliable. One solution could be to wait until the end of training, then run the whole training set through the neural network and compute the mean and standard deviation of each input of the BN layer. These "final" input means and standard deviations could then be used instead of the batch input means and standard deviations when making predictions. However, most implementations of Batch Normalization estimate these final statistics during training by using a moving average of the layer's input means and standard deviations. This is what Keras does automatically when you use the `BatchNormalization` layer. To sum up, four parameter vectors are learned in each batch-normalized layer: $\boldsymbol{\gamma}$ (the output scale vector) and $\boldsymbol{\beta}$

(the output offset vector) are learned through regular backpropagation, and **μ** (the final input mean vector) and **σ** (the final input standard deviation vector) are estimated using an exponential moving average. Note that **μ** and **σ** are estimated during training, but they are used only after training (to replace the batch input means and standard deviations in Equation 11-4).

Ioffe and Szegedy demonstrated that Batch Normalization considerably improved all the deep neural networks they experimented with, leading to a huge improvement in the ImageNet classification task (ImageNet is a large database of images classified into many classes, commonly used to evaluate computer vision systems). The vanishing gradients problem was strongly reduced, to the point that they could use saturating activation functions such as the tanh and even the sigmoid activation function. The networks were also much less sensitive to the weight initialization. The authors were able to use much larger learning rates, significantly speeding up the learning process. Specifically, they note that:

> *Applied to a state-of-the-art image classification model, Batch Normalization achieves the same accuracy with 14 times fewer training steps, and beats the original model by a significant margin. […] Using an ensemble of batch-normalized networks, we improve upon the best published result on ImageNet classification: reaching 4.9% top-5 validation error (and 4.8% test error), exceeding the accuracy of human raters.*

Finally, like a gift that keeps on giving, Batch Normalization acts like a regularizer, reducing the need for other regularization techniques (such as dropout, described later in this chapter).

Batch Normalization does, however, add some complexity to the model (although it can remove the need for normalizing the input data, as we discussed earlier). Moreover, there is a runtime penalty: the neural network makes slower predictions due to the extra computations required at each layer. Fortunately, it's often possible to fuse the BN layer with the previous layer, after training, thereby avoiding the runtime penalty. This is done by updating the previous layer's weights and biases so that it directly produces outputs of the appropriate scale and offset. For example, if the previous layer computes $\mathbf{XW} + \mathbf{b}$, then the BN layer will compute $\boldsymbol{\gamma} \otimes (\mathbf{XW} + \mathbf{b} - \boldsymbol{\mu}) / \boldsymbol{\sigma} + \boldsymbol{\beta}$ (ignoring the smoothing term ε in the denominator). If we define $\mathbf{W}' = \boldsymbol{\gamma} \otimes$*W*/$\boldsymbol{\sigma}$ and $\mathbf{b}' = \boldsymbol{\gamma} \otimes (\mathbf{b} - \boldsymbol{\mu}) / \boldsymbol{\sigma} + \boldsymbol{\beta}$, the equation simplifies to $\mathbf{XW}' + \mathbf{b}'$. So if we replace the previous layer's weights and biases ($\mathbf{W}$ and $\mathbf{b}$) with the updated weights and biases ($\mathbf{W}'$ and $\mathbf{b}'$), we can get rid of the BN layer (TFLite's converter does this automatically; see Chapter 19).

> **NOTE**
>
> You may find that training is rather slow, because each epoch takes much more time when you use Batch Normalization. This is usually counterbalanced by the fact that convergence is much faster with BN, so it will take fewer epochs to reach the same performance. All in all, *wall time* will usually be shorter (this is the time measured by the clock on your wall).

Implementing Batch Normalization with Keras

As with most things with Keras, implementing Batch Normalization is straightforward and intuitive. Just add a `BatchNormalization` layer before or after each hidden layer's activation function, and optionally add a BN layer as well as the first layer in your model. For example, this model applies BN after every hidden layer and as the first layer in the model (after flattening the input images):

```
model = tf.keras.Sequential([
    tf.keras.layers.Flatten(input_shape=[28, 28]),
    tf.keras.layers.BatchNormalization(),
    tf.keras.layers.Dense(300, activation="relu",
                          kernel_initializer="he_normal"),
    tf.keras.layers.BatchNormalization(),
    tf.keras.layers.Dense(100, activation="relu",
                          kernel_initializer="he_normal"),
    tf.keras.layers.BatchNormalization(),
    tf.keras.layers.Dense(10, activation="softmax")
])
```

That's all! In this tiny example with just two hidden layers, Batch Normalization is unlikely to have a large impact, but for deeper networks it can make a tremendous difference.

Let’s display the model summary:

```
>>> model.summary()
Model: "sequential"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
flatten (Flatten)            (None, 784)               0
_________________________________________________________________
batch_normalization (BatchNo (None, 784)               3136
_________________________________________________________________
dense (Dense)                (None, 300)               235500
_________________________________________________________________
batch_normalization_1 (Batch (None, 300)               1200
_________________________________________________________________
dense_1 (Dense)              (None, 100)               30100
_________________________________________________________________
batch_normalization_2 (Batch (None, 100)               400
_________________________________________________________________
dense_2 (Dense)              (None, 10)                1010
=================================================================
Total params: 271,346
Trainable params: 268,978
Non-trainable params: 2,368
_________________________________________________________________
```

As you can see, each BN layer adds four parameters per input: **γ**, **β**, **μ**, and **σ** (for example, the first BN layer adds 3,136 parameters, which is 4 × 784). The last two parameters, **μ** and **σ**, are the moving averages; they are not affected by backpropagation, so Keras calls them “non-trainable"[13] (if you count the total number of BN parameters, 3,136 + 1,200 + 400, and divide by 2, you get 2,368, which is the total number of non-trainable parameters in this model).

Let’s look at the parameters of the first BN layer. Two are trainable (by backpropagation), and two are not:

```
>>> [(var.name, var.trainable) for var in
model.layers[1].variables]
[('batch_normalization/gamma:0', True),
 ('batch_normalization/beta:0', True),
```

```
('batch_normalization/moving_mean:0', False),
('batch_normalization/moving_variance:0', False)]
```

The authors of the BN paper argued in favor of adding the BN layers before the activation functions, rather than after (as we just did). There is some debate about this, as which is preferable seems to depend on the task—you can experiment with this too to see which option works best on your dataset. To add the BN layers before the activation functions, you must remove the activation function from the hidden layers and add them as separate layers after the BN layers. Moreover, since a Batch Normalization layer includes one offset parameter per input, you can remove the bias term from the previous layer by passing `use_bias=False` when creating it. And lastly, you can usually drop the first BN layer to avoid sandwitching the first hidden layer between two BN layers. The updated code looks like this:

```
model = tf.keras.Sequential([
    tf.keras.layers.Flatten(input_shape=[28, 28]),
    tf.keras.layers.Dense(300, kernel_initializer="he_normal",
use_bias=False),
    tf.keras.layers.BatchNormalization(),
    tf.keras.layers.Activation("relu"),
    tf.keras.layers.Dense(100, kernel_initializer="he_normal",
use_bias=False),
    tf.keras.layers.BatchNormalization(),
    tf.keras.layers.Activation("relu"),
    tf.keras.layers.Dense(10, activation="softmax")
])
```

The `BatchNormalization` class has quite a few hyperparameters you can tweak. The defaults will usually be fine, but you may occasionally need to tweak the `momentum`. This hyperparameter is used by the `BatchNormalization` layer when it updates the exponential moving averages; given a new value **v** (i.e., a new vector of input means or standard deviations computed over the current batch), the layer updates the running average $\widehat{\mathbf{v}}$ using the following equation:

$$\widehat{\mathbf{v}} \leftarrow \widehat{\mathbf{v}} \times \text{momentum} + \mathbf{v} \times (1 - \text{momentum})$$

A good momentum value is typically close to 1; for example, 0.9, 0.99, or 0.999. You want more 9s for larger datasets and for smaller mini-batches.

Another important hyperparameter is `axis`: it determines which axis should be normalized. It defaults to –1, meaning that by default it will normalize the last axis (using the means and standard deviations computed across the *other* axes). When the input batch is 2D (i.e., the batch shape is [*batch size, features*]), this means that each input feature will be normalized based on the mean and standard deviation computed across all the instances in the batch. For example, the first BN layer in the previous code example will independently normalize (and rescale and shift) each of the 784 input features. If we move the first BN layer before the `Flatten` layer, then the input batches will be 3D, with shape [*batch size, height, width*]; therefore, the BN layer will compute 28 means and 28 standard deviations (1 per column of pixels, computed across all instances in the batch and across all rows in the column), and it will normalize all pixels in a given column using the same mean and standard deviation. There will also be just 28 scale parameters and 28 shift parameters. If instead you still want to treat each of the 784 pixels independently, then you should set `axis=[1, 2]`.

Batch Normalization has become one of the most-used layers in deep neural networks, especially deep convolutional neural networks (Chapter 14), to the point that it is often omitted in the architecture diagrams: it is assumed that BN is added after every layer. Now let's look at one last technique to stabilize gradients during training: Gradient Clipping.

Gradient Clipping

Another popular technique to mitigate the exploding gradients problem is to clip the gradients during backpropagation so that they never exceed some threshold. This is called *Gradient Clipping*.[14] This technique is most often used in recurrent neural networks, as Batch Normalization is tricky to use in RNNs, as we will see in Chapter 16.

In Keras, implementing Gradient Clipping is just a matter of setting the `clipvalue` or `clipnorm` argument when creating an optimizer, like this:

```
optimizer = tf.keras.optimizers.SGD(clipvalue=1.0)
model.compile([...], optimizer=optimizer)
```

This optimizer will clip every component of the gradient vector to a value between –1.0 and 1.0. This means that all the partial derivatives of the loss (with regard to each and every trainable parameter) will be clipped between –1.0 and 1.0. The threshold is a hyperparameter you can tune. Note that it may change the orientation of the gradient vector. For instance, if the original gradient vector is [0.9, 100.0], it points mostly in the direction of the second axis; but once you clip it by value, you get [0.9, 1.0], which points roughly in the diagonal between the two axes. In practice, this approach works well. If you want to ensure that Gradient Clipping does not change the direction of the gradient vector, you should clip by norm by setting `clipnorm` instead of `clipvalue`. This will clip the whole gradient if its ℓ_2 norm is greater than the threshold you picked. For example, if you set `clipnorm=1.0`, then the vector [0.9, 100.0] will be clipped to [0.00899964, 0.9999595], preserving its orientation but almost eliminating the first component. If you observe that the gradients explode during training (you can track the size of the gradients using TensorBoard), you may want to try clipping by value or clipping by norm, with different thresholds, and see which option performs best on the validation set.

Reusing Pretrained Layers

It is generally not a good idea to train a very large DNN from scratch without first trying to find an existing neural network that accomplishes a similar task to the one you are trying to tackle (we will discuss how to find them in Chapter 14). If you find such as neural network, then you can generally reuse most of its layers, except for the top ones. This technique is called *transfer learning*. It will not only speed up training considerably, but also require significantly less training data.

Suppose you have access to a DNN that was trained to classify pictures into 100 different categories, including animals, plants, vehicles, and everyday objects. You now want to train a DNN to classify specific types of vehicles. These tasks are very similar, even partly overlapping, so you should try to reuse parts of the first network (see Figure 11-5).

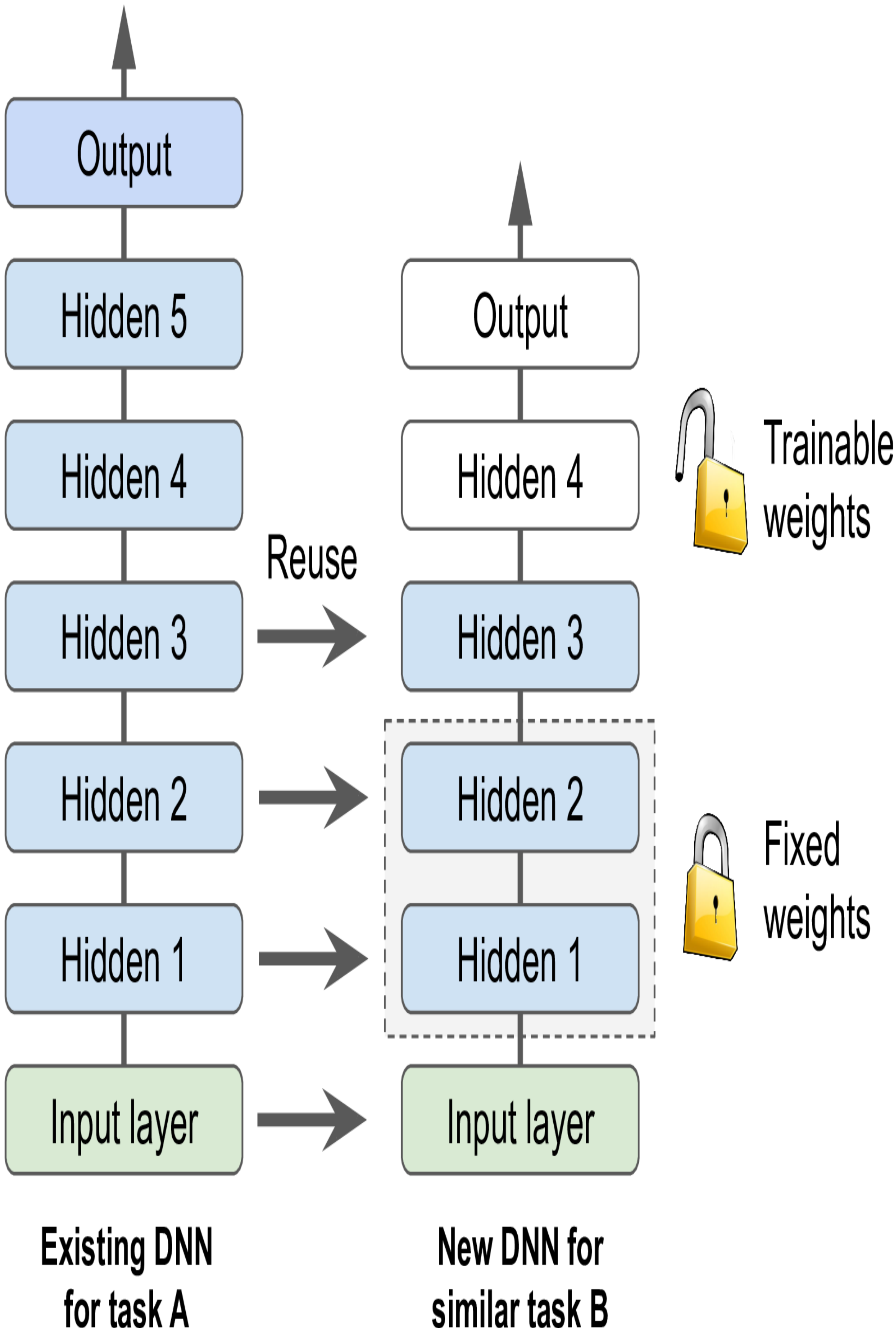

Output
Hidden 5
Hidden 4
Hidden 3
Hidden 2
Hidden 1
Input layer
Reuse
Output
Hidden 4
Hidden 3
Hidden 2
Hidden 1
Input layer
Trainable weights
Fixed weights
Existing DNN for task A
New DNN for similar task B

Figure 11-5. Reusing pretrained layers

> **NOTE**
>
> If the input pictures of your new task don't have the same size as the ones used in the original task, you will usually have to add a preprocessing step to resize them to the size expected by the original model. More generally, transfer learning will work best when the inputs have similar low-level features.

The output layer of the original model should usually be replaced because it is most likely not useful at all for the new task, and it generally does not even have the right number of outputs.

Similarly, the upper hidden layers of the original model are less likely to be as useful as the lower layers, since the high-level features that are most useful for the new task may differ significantly from the ones that were most useful for the original task. You want to find the right number of layers to reuse.

> **TIP**
>
> The more similar the tasks are, the more layers you want to reuse (starting with the lower layers). For very similar tasks, try to keep all the hidden layers and just replace the output layer.

Try freezing all the reused layers first (i.e., make their weights non-trainable so that Gradient Descent won't modify them), then train your model and see how it performs. Then try unfreezing one or two of the top hidden layers to let backpropagation tweak them and see if performance improves. The more training data you have, the more layers you can unfreeze. It is also useful to reduce the learning rate when you unfreeze reused layers: this will avoid wrecking their fine-tuned weights.

If you still cannot get good performance, and you have little training data, try dropping the top hidden layer(s) and freezing all the remaining hidden layers again. You can iterate until you find the right number of layers to reuse. If you have plenty of training data, you may try replacing the top hidden layers instead of dropping them, and even adding more hidden layers.

Transfer Learning with Keras

Let's look at an example. Suppose the Fashion MNIST dataset only contained eight classes—for example, all the classes except for sandal and shirt. Someone built and trained a Keras model on that set and got reasonably good performance (>90% accuracy). Let's call this model A. You now want to tackle a different task: you have images of T-shirts and pullovers, and you want to train a binary classifier: positive for T-shirts (and tops), negative for sandals. Your dataset is quite small; you only have 200 labeled images. When you train a new model for this task (let's call it model B) with the same architecture as model A, you get 91.85% test accuracy. While drinking your morning coffee, you realize that your task is quite similar to task A, so perhaps transfer learning can help? Let's find out!

First, you need to load model A and create a new model based on that model's layers. Let's reuse all the layers except for the output layer:

```
[...]  # Assuming model A was already trained and saved to
"my_model_A"
model_A = tf.keras.models.load_model("my_model_A")
model_B_on_A = tf.keras.Sequential(model_A.layers[:-1])
model_B_on_A.add(tf.keras.layers.Dense(1, activation="sigmoid"))
```

Note that `model_A` and `model_B_on_A` now share some layers. When you train `model_B_on_A`, it will also affect `model_A`. If you want to avoid that, you need to *clone* `model_A` before you reuse its layers. To do this, you clone model A's architecture with `clone_model()`, then copy its weights:

```
model_A_clone = tf.keras.models.clone_model(model_A)
model_A_clone.set_weights(model_A.get_weights())
```

WARNING

`tf.keras.models.clone_model()` only clones the architecture, not the weights. If you don't copy them manually using `set_weights()`, they will be initialized randomly when the cloned model is first used.

Now you could train `model_B_on_A` for task B, but since the new output layer was initialized randomly it will make large errors (at least during the first few epochs), so there will be large error gradients that may wreck the reused weights. To avoid this, one approach is to freeze the reused layers during the first few epochs, giving the new layer some time to learn reasonable weights. To do this, set every layer's `trainable` attribute to `False` and compile the model:

```
for layer in model_B_on_A.layers[:-1]:
    layer.trainable = False

optimizer = tf.keras.optimizers.SGD(learning_rate=0.001)
model_B_on_A.compile(loss="binary_crossentropy",
optimizer=optimizer,
                     metrics=["accuracy"])
```

NOTE

You must always compile your model after you freeze or unfreeze layers.

Now you can train the model for a few epochs, then unfreeze the reused layers (which requires compiling the model again) and continue training to fine-tune the reused layers for task B. After unfreezing the reused layers, it is usually a good idea to reduce the learning rate, once again to avoid damaging the reused weights.

```
history = model_B_on_A.fit(X_train_B, y_train_B, epochs=4,
                           validation_data=(X_valid_B,
y_valid_B))
```

```
for layer in model_B_on_A.layers[:-1]:
    layer.trainable = True

optimizer = tf.keras.optimizers.SGD(learning_rate=0.001)
model_B_on_A.compile(loss="binary_crossentropy",
optimizer=optimizer,
                     metrics=["accuracy"])
history = model_B_on_A.fit(X_train_B, y_train_B, epochs=16,
                           validation_data=(X_valid_B,
y_valid_B))
```

So, what’s the final verdict? Well, this model’s test accuracy is 93.85%, up exactly two percentage points from 91.85%! This means that transfer learning reduced the error rate by almost 25%!

```
>>> model_B_on_A.evaluate(X_test_B, y_test_B)
[0.2546142041683197, 0.9384999871253967]
```

Are you convinced? You shouldn’t be: I cheated! I tried many configurations until I found one that demonstrated a strong improvement. If you try to change the classes or the random seed, you will see that the improvement generally drops, or even vanishes or reverses. What I did is called “torturing the data until it confesses.” When a paper just looks too positive, you should be suspicious: perhaps the flashy new technique does not actually help much (in fact, it may even degrade performance), but the authors tried many variants and reported only the best results (which may be due to sheer luck), without mentioning how many failures they encountered on the way. Most of the time, this is not malicious at all, but it is part of the reason so many results in science can never be reproduced.

Why did I cheat? It turns out that transfer learning does not work very well with small dense networks, presumably because small networks learn few patterns, and dense networks learn very specific patterns, which are unlikely to be useful in other tasks. Transfer learning works best with deep convolutional neural networks, which tend to learn feature detectors that are much more general (especially in the lower layers). We will revisit transfer learning in Chapter 14, using the techniques we just discussed (and this time there will be no cheating, I promise!).

Unsupervised Pretraining

Suppose you want to tackle a complex task for which you don't have much labeled training data, but unfortunately you cannot find a model trained on a similar task. Don't lose hope! First, you should try to gather more labeled training data, but if you can't, you may still be able to perform *unsupervised pretraining* (see Figure 11-6). Indeed, it is often cheap to gather unlabeled training examples, but expensive to label them. If you can gather plenty of unlabeled training data, you can try to use it to train an unsupervised model, such as an autoencoder or a generative adversarial network (see Chapter 17). Then you can reuse the lower layers of the autoencoder or the lower layers of the GAN's discriminator, add the output layer for your task on top, and fine-tune the final network using supervised learning (i.e., with the labeled training examples).

It is this technique that Geoffrey Hinton and his team used in 2006 and which led to the revival of neural networks and the success of Deep Learning. Until 2010, unsupervised pretraining—typically with restricted Boltzmann machines (RBMs; see the notebook at *https://homl.info/extra-anns*)—was the norm for deep nets, and only after the vanishing gradients problem was alleviated did it become much more common to train DNNs purely using supervised learning. Unsupervised pretraining (today typically using autoencoders or GANs rather than RBMs) is still a good option when you have a complex task to solve, no similar model you can reuse, and little labeled training data but plenty of unlabeled training data.

Note that in the early days of Deep Learning it was difficult to train deep models, so people would use a technique called *greedy layer-wise pretraining* (depicted in Figure 11-6). They would first train an unsupervised model with a single layer, typically an RBM, then they would freeze that layer and add another one on top of it, then train the model again (effectively just training the new layer), then freeze the new layer and add another layer on top of it, train the model again, and so on. Nowadays, things are much simpler: people generally train the full unsupervised model in one shot (i.e., in Figure 11-6, just start directly at step three) and use autoencoders or GANs rather than RBMs.

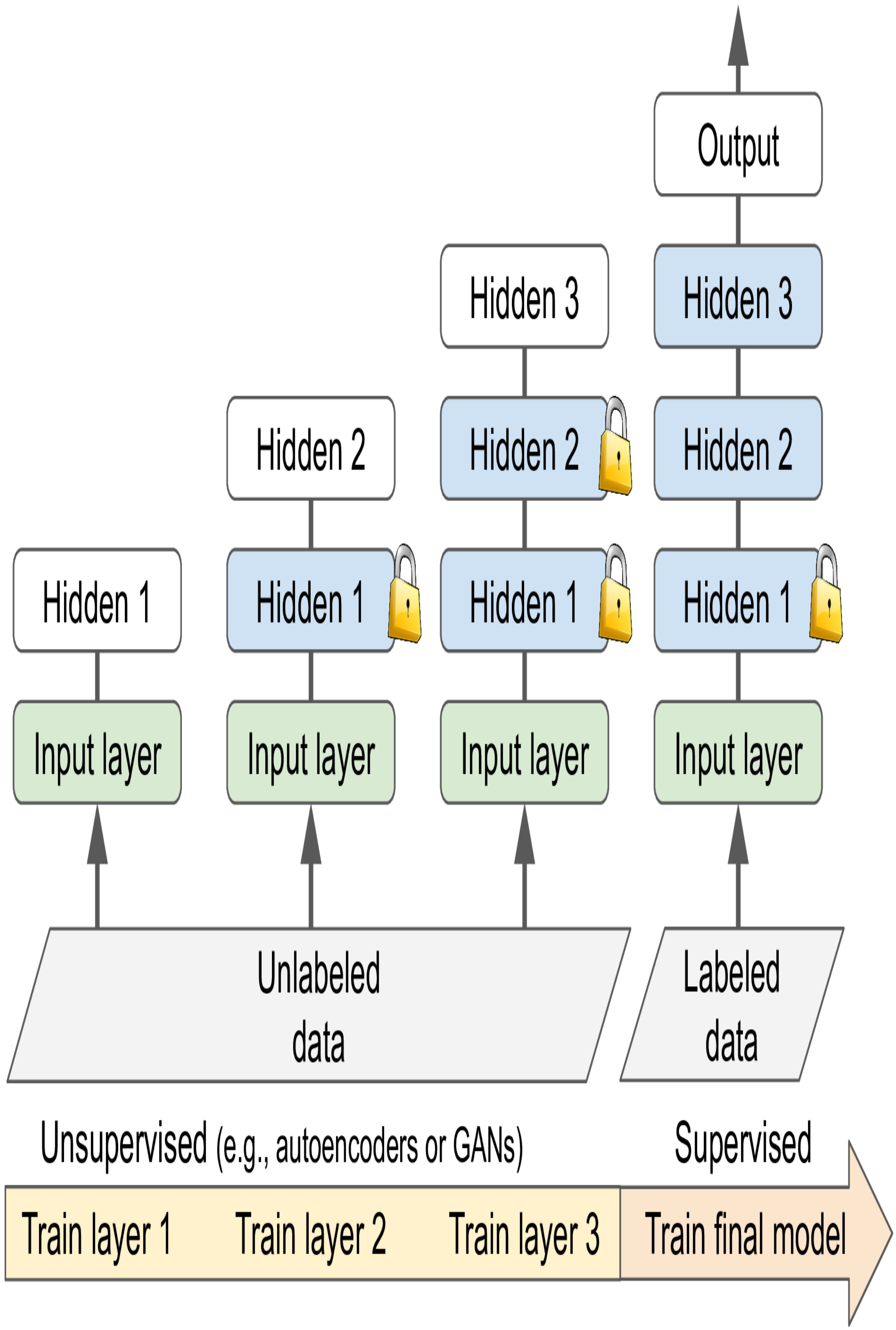

Output
Hidden 3
Hidden 3
Hidden 2
Hidden 2
Hidden 2
Hidden 1
Hidden 1
Hidden 1
Hidden 1
Input layer
Input layer
Input layer
Input layer
Unlabeled data
Labeled data
Unsupervised (e.g., autoencoders or GANs)
Supervised
Train layer 1
Train layer 2
Train layer 3
Train final model

Figure 11-6. In unsupervised training, a model is trained on all data, including the unlabeled data, using an unsupervised learning technique, then it is fine-tuned for the final task on just the labeled data using a supervised learning technique; the unsupervised part may train one layer at a time as shown here, or it may train the full model directly

Pretraining on an Auxiliary Task

If you do not have much labeled training data, one last option is to train a first neural network on an auxiliary task for which you can easily obtain or generate labeled training data, then reuse the lower layers of that network for your actual task. The first neural network's lower layers will learn feature detectors that will likely be reusable by the second neural network.

For example, if you want to build a system to recognize faces, you may only have a few pictures of each individual—clearly not enough to train a good classifier. Gathering hundreds of pictures of each person would not be practical. You could, however, gather a lot of pictures of random people on the web and train a first neural network to detect whether or not two different pictures feature the same person. Such a network would learn good feature detectors for faces, so reusing its lower layers would allow you to train a good face classifier that uses little training data.

For *natural language processing* (NLP) applications, you can download a corpus of millions of text documents and automatically generate labeled data from it. For example, you could randomly mask out some words and train a model to predict what the missing words are (e.g., it should predict that the missing word in the sentence "What ___ you saying?" is probably "are" or "were"). If you can train a model to reach good performance on this task, then it will already know quite a lot about language, and you can certainly reuse it for your actual task and fine-tune it on your labeled data (we will discuss more pretraining tasks in Chapter 16).

> **NOTE**
>
> *Self-supervised learning* is when you automatically generate the labels from the data itself, as in the text-masking example, then you train a model on the resulting "labeled" dataset using supervised learning techniques.

Faster Optimizers

Training a very large deep neural network can be painfully slow. So far we have seen four ways to speed up training (and reach a better solution): applying a good initialization strategy for the connection weights, using a good activation function, using Batch Normalization, and reusing parts of a pretrained network (possibly built on an auxiliary task or using unsupervised learning). Another huge speed boost comes from using a faster optimizer than the regular Gradient Descent optimizer. In this section we will present the most popular algorithms: momentum optimization, Nesterov Accelerated Gradient, AdaGrad, RMSProp, and finally Adam optimization and its variants.

Momentum Optimization

Imagine a bowling ball rolling down a gentle slope on a smooth surface: it will start out slowly, but it will quickly pick up momentum until it eventually reaches terminal velocity (if there is some friction or air resistance). This is the core idea of *momentum optimization*, proposed by Boris Polyak in 1964.[15] In contrast, regular Gradient Descent will take small steps when the slope is gentle, and big steps when the slope is steep, but it will never pick up speed. As a result, regular Gradient Descent is generally much slower to reach the minimum than momentum optimization.

Recall that Gradient Descent updates the weights $\boldsymbol{\theta}$ by directly subtracting the gradient of the cost function $J(\boldsymbol{\theta})$ with regard to the weights ($\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$) multiplied by the learning rate η. The equation is: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$. It does not care about what the earlier gradients were. If the local gradient is tiny, it goes very slowly.

Momentum optimization cares a great deal about what previous gradients were: at each iteration, it subtracts the local gradient from the *momentum vector* **m** (multiplied by the learning rate η), and it updates the weights by adding this momentum vector (see Equation 11-5). In other words, the gradient is used as an acceleration, not as a speed. To simulate some sort of friction mechanism and prevent the momentum from growing too large, the algorithm introduces a new hyperparameter β, called the *momentum*, which must be set between 0 (high friction) and 1 (no friction). A typical momentum value is 0.9.

Equation 11-5. Momentum algorithm

$$
\begin{aligned}
1. \quad & \mathbf{m} \leftarrow \beta \mathbf{m} - \eta \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \\
2. \quad & \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \mathbf{m}
\end{aligned}
$$

You can verify that if the gradient remains constant, the terminal velocity (i.e., the maximum size of the weight updates) is equal to that gradient multiplied by the learning rate η multiplied by $1 / (1 - \beta)$ (ignoring the sign). For example, if $\beta = 0.9$, then the terminal velocity is equal to 10 times the gradient times the learning rate, so momentum optimization ends up going 10 times faster than Gradient Descent! This allows momentum optimization to escape from plateaus much faster than Gradient Descent. We saw in Chapter 4 that when the inputs have very different scales, the cost function will look like an elongated bowl (see Figure 4-7). Gradient Descent goes down the steep slope quite fast, but then it takes a very long time to go down the valley. In contrast, momentum optimization will roll down the valley faster and faster until it reaches the bottom (the optimum). In deep neural networks that don't use Batch Normalization, the upper layers will often end up having inputs with very different scales, so using momentum optimization helps a lot. It can also help roll past local optima.

NOTE

Due to the momentum, the optimizer may overshoot a bit, then come back, overshoot again, and oscillate like this many times before stabilizing at the minimum. This is one of the reasons it's good to have a bit of friction in the system: it gets rid of these oscillations and thus speeds up convergence.

Implementing momentum optimization in Keras is a no-brainer: just use the `SGD` optimizer and set its `momentum` hyperparameter, then lie back and profit!

```
optimizer = tf.keras.optimizers.SGD(learning_rate=0.001,
momentum=0.9)
```

The one drawback of momentum optimization is that it adds yet another hyperparameter to tune. However, the momentum value of 0.9 usually works well in practice and almost always goes faster than regular Gradient Descent.

Nesterov Accelerated Gradient

One small variant to momentum optimization, proposed by Yurii Nesterov in 1983,[16] is almost always faster than regular momentum optimization. The *Nesterov Accelerated Gradient* (NAG) method, also known as *Nesterov momentum optimization*, measures the gradient of the cost function not at the local position $\boldsymbol{\theta}$ but slightly ahead in the direction of the momentum, at $\boldsymbol{\theta} + \beta\mathbf{m}$ (see Equation 11-6).

Equation 11-6. Nesterov Accelerated Gradient algorithm

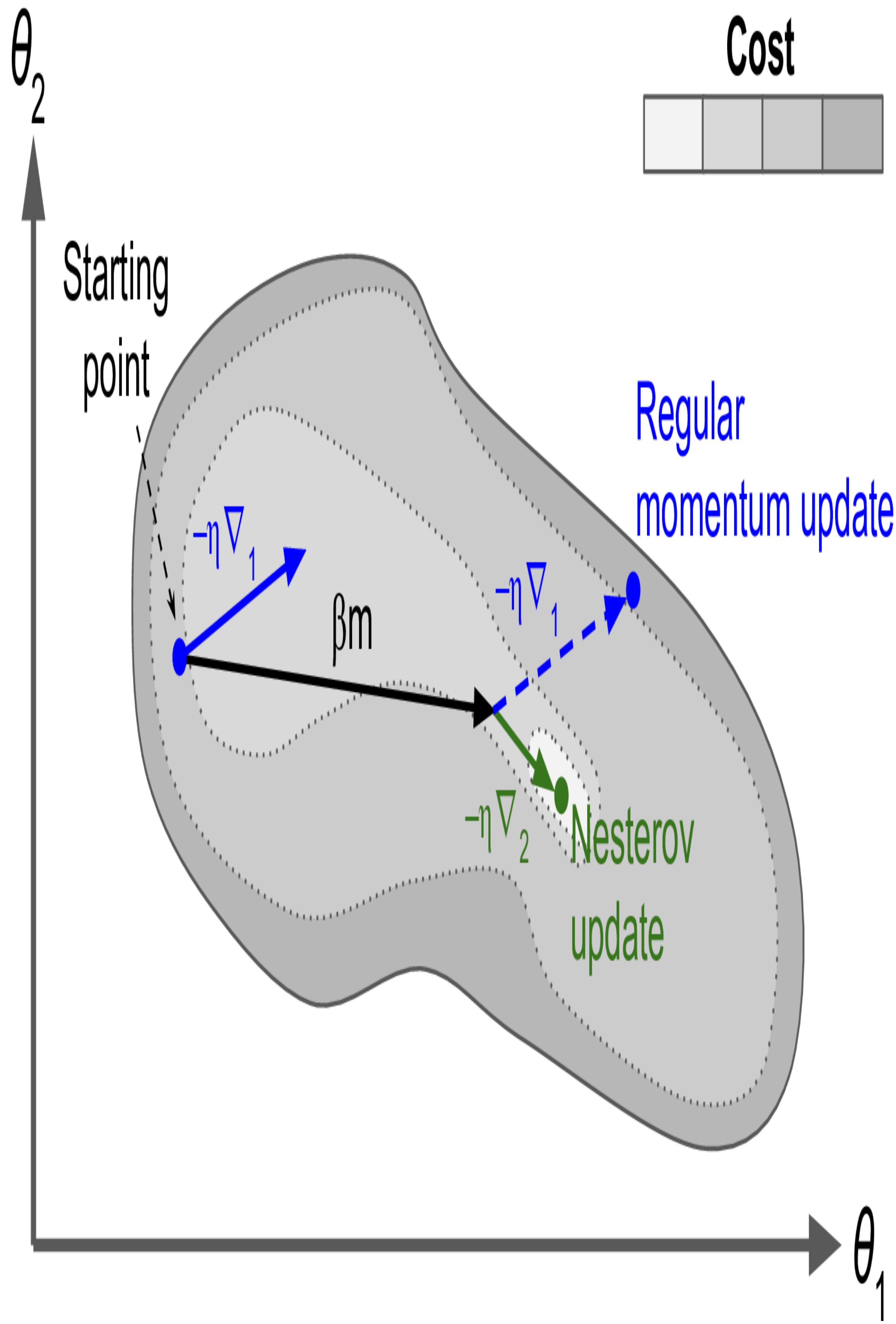
$$\begin{aligned} 1. \quad & \mathbf{m} \leftarrow \beta\mathbf{m} - \eta \nabla_{\boldsymbol{\theta}} J\left(\boldsymbol{\theta} + \beta\mathbf{m}\right) \\ 2. \quad & \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \mathbf{m} \end{aligned}$$

This small tweak works because in general the momentum vector will be pointing in the right direction (i.e., toward the optimum), so it will be slightly more accurate to use the gradient measured a bit farther in that direction rather than the gradient at the original position, as you can see in Figure 11-7 (where ∇_1 represents the gradient of the cost function measured at the starting point $\boldsymbol{\theta}$, and ∇_2 represents the gradient at the point located at $\boldsymbol{\theta} + \beta\mathbf{m}$).

As you can see, the Nesterov update ends up closer to the optimum. After a while, these small improvements add up and NAG ends up being significantly faster than regular momentum optimization. Moreover, note that when the momentum pushes the weights across a valley, ∇_1 continues to push farther across the valley, while ∇_2 pushes back toward the bottom of the valley. This helps reduce oscillations and thus NAG converges faster.

NAG is generally faster than regular momentum optimization. To use it, simply set `nesterov=True` when creating the `SGD` optimizer:

```
optimizer = tf.keras.optimizers.SGD(learning_rate=0.001,
momentum=0.9,
                                    nesterov=True)
```



θ2
Cost
Starting point
Regular momentum update
−η∇1
βm
−η∇1
−η∇2
Nesterov update
θ1

Figure 11-7. Regular versus Nesterov momentum optimization: the former applies the gradients computed before the momentum step, while the latter applies the gradients computed after

AdaGrad

Consider the elongated bowl problem again: Gradient Descent starts by quickly going down the steepest slope, which does not point straight toward the global optimum, then it very slowly goes down to the bottom of the valley. It would be nice if the algorithm could correct its direction earlier to point a bit more toward the global optimum. The *AdaGrad* algorithm[17] achieves this correction by scaling down the gradient vector along the steepest dimensions (see Equation 11-7).

Equation 11-7. AdaGrad algorithm

$$
\begin{aligned}
&1. \quad \mathbf{s} \leftarrow \mathbf{s} + \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \otimes \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \\
&2. \quad \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \oslash \sqrt{\mathbf{s} + \varepsilon}
\end{aligned}
$$

The first step accumulates the square of the gradients into the vector **s** (recall that the $\otimes$ symbol represents the element-wise multiplication). This vectorized form is equivalent to computing $s_i \leftarrow s_i + (\partial J(\boldsymbol{\theta}) / \partial \theta_i)^2$ for each element s_i of the vector **s**; in other words, each s_i accumulates the squares of the partial derivative of the cost function with regard to parameter θ_i. If the cost function is steep along the i^{th} dimension, then s_i will get larger and larger at each iteration.

The second step is almost identical to Gradient Descent, but with one big difference: the gradient vector is scaled down by a factor of $\sqrt{\mathbf{s} + \varepsilon}$ (the $\oslash$ symbol represents the element-wise division, and ε is a smoothing term to avoid division by zero, typically set to 10^{-10}). This vectorized form is equivalent to simultaneously computing $\theta_i \leftarrow \theta_i - \eta\, \partial J(\boldsymbol{\theta}) / \partial \theta_i / \sqrt{s_i + \varepsilon}$ for all parameters θ_i.

In short, this algorithm decays the learning rate, but it does so faster for steep dimensions than for dimensions with gentler slopes. This is called an *adaptive learning rate*. It helps point the resulting updates more directly toward the global optimum (see Figure 11-8). One additional benefit is that it requires much less tuning of the learning rate hyperparameter η.

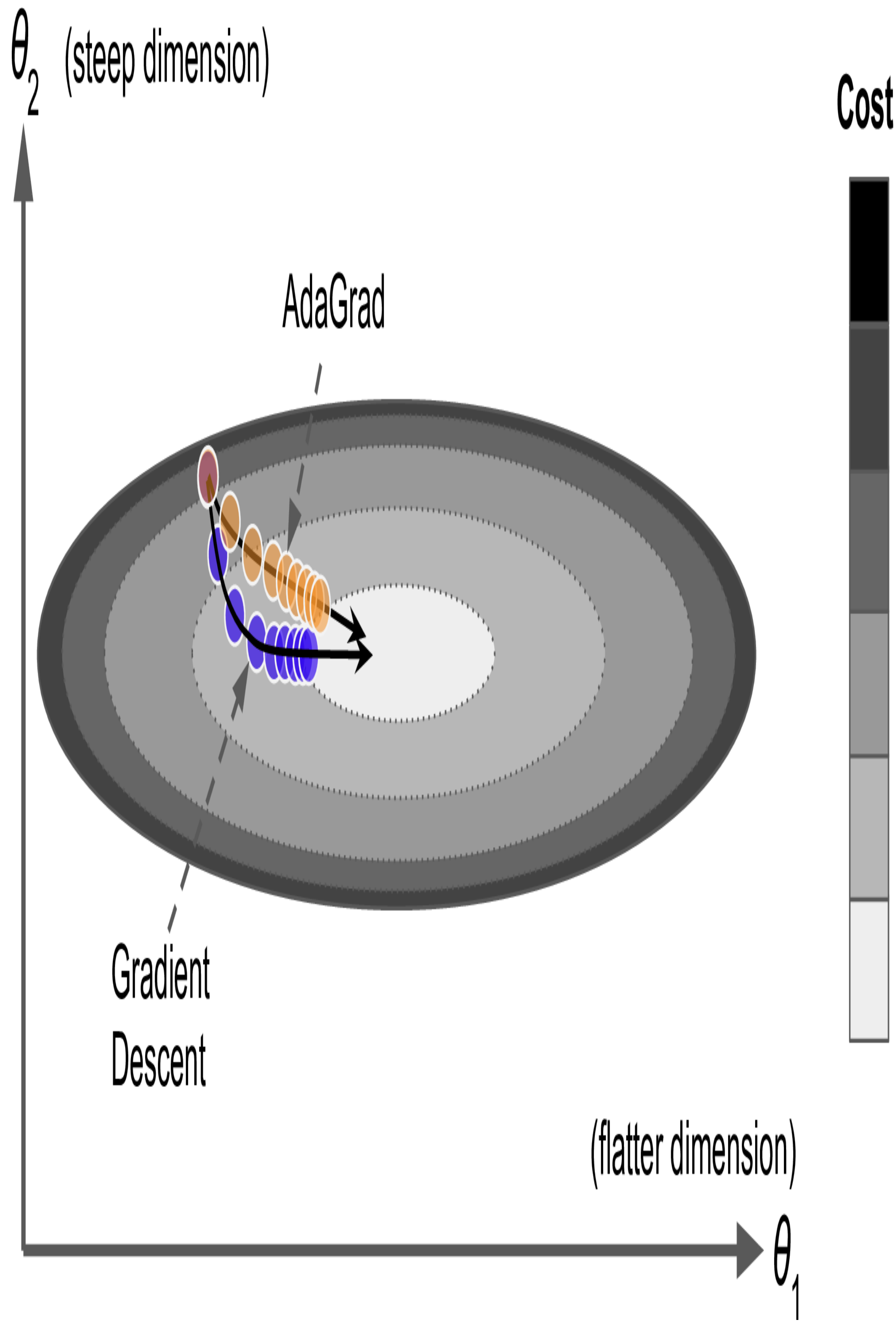

θ_2 (steep dimension)
Cost
AdaGrad
Gradient
Descent
(flatter dimension)
θ_1

Figure 11-8. AdaGrad versus Gradient Descent: the former can correct its direction earlier to point to the optimum

AdaGrad frequently performs well for simple quadratic problems, but it often stops too early when training neural networks. The learning rate gets scaled down so much that the algorithm ends up stopping entirely before reaching the global optimum. So even though Keras has an `Adagrad` optimizer, you should not use it to train deep neural networks (it may be efficient for simpler tasks such as Linear Regression, though). Still, understanding AdaGrad is helpful to grasp the other adaptive learning rate optimizers.

RMSProp

As we've seen, AdaGrad runs the risk of slowing down a bit too fast and never converging to the global optimum. The *RMSProp* algorithm[18] fixes this by accumulating only the gradients from the most recent iterations, as opposed to all the gradients since the beginning of training. It does so by using exponential decay in the first step (see Equation 11-8).

Equation 11-8. RMSProp algorithm

$$\begin{aligned} &1. \quad \mathbf{s} \leftarrow \rho\mathbf{s} + (1-\rho)\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \otimes \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \\ &2. \quad \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \oslash \sqrt{\mathbf{s}+\varepsilon} \end{aligned}$$

The decay rate ρis typically set to 0.9.[19] Yes, it is once again a new hyperparameter, but this default value often works well, so you may not need to tune it at all.

As you might expect, Keras has an `RMSprop` optimizer:

```
optimizer = tf.keras.optimizers.RMSprop(learning_rate=0.001,
rho=0.9)
```

Except on very simple problems, this optimizer almost always performs much better than AdaGrad. In fact, it was the preferred optimization algorithm of many researchers until Adam optimization came around.

Adam Optimization

Adam,[20] which stands for *adaptive moment estimation*, combines the ideas of momentum optimization and RMSProp: just like momentum optimization, it keeps track of an exponentially decaying average of past gradients; and just like RMSProp, it keeps track of an exponentially decaying average of past squared gradients (see Equation 11-9). These are estimations of the mean and (uncentered) variance of the gradients. The mean is often called the *first moment* while the variance is often called the *second moment*, hence the name of the algorithm.

Equation 11-9. Adam algorithm

$$
\begin{aligned}
1.\quad & \mathbf{m} \leftarrow \beta_1 \mathbf{m} - (1-\beta_1) \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \\
2.\quad & \mathbf{s} \leftarrow \beta_2 \mathbf{s} + (1-\beta_2) \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \otimes \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \\
3.\quad & \widehat{\mathbf{m}} \leftarrow \frac{\mathbf{m}}{1-{\beta_1}^t} \\
4.\quad & \hat{\mathbf{s}} \leftarrow \frac{\mathbf{s}}{1-{\beta_2}^t} \\
5.\quad & \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \eta \widehat{\mathbf{m}} \oslash \sqrt{\hat{\mathbf{s}} + \varepsilon}
\end{aligned}
$$

In this equation, t represents the iteration number (starting at 1).

If you just look at steps 1, 2, and 5, you will notice Adam's close similarity to both momentum optimization and RMSProp: β_1 corresponds to β in momentum optimization, and β_2 corresponds to ρin RMSProp. The only difference is that step 1 computes an exponentially decaying average rather than an exponentially decaying sum, but these are actually equivalent except for a constant factor (the decaying average is just $1 - \beta_1$ times the decaying sum). Steps 3 and 4 are somewhat of a technical detail: since **m** and **s** are initialized at 0, they will be biased toward 0 at the beginning of training, so these two steps will help boost **m** and **s** at the beginning of training.

The momentum decay hyperparameter β_1 is typically initialized to 0.9, while the scaling decay hyperparameter β_2 is often initialized to 0.999. As earlier, the smoothing term ε is usually initialized to a tiny number such as 10^{-7}. These are the default values for the `Adam` class. Here is how to create an Adam optimizer using Keras:

```
optimizer = tf.keras.optimizers.Adam(learning_rate=0.001,
beta_1=0.9,
                                     beta_2=0.999)
```

Since Adam is an adaptive learning rate algorithm, like AdaGrad and RMSProp, it requires less tuning of the learning rate hyperparameter η. You can often use the default value $\eta = 0.001$, making Adam even easier to use than Gradient Descent.

> **TIP**
>
> If you are starting to feel overwhelmed by all these different techniques and are wondering how to choose the right ones for your task, don't worry: some practical guidelines are provided at the end of this chapter.

Finally, three variants of Adam are worth mentioning:

AdaMax

The Adam paper also introduced AdaMax. Notice that in step 2 of Equation 11-9, Adam accumulates the squares of the gradients in **s** (with a greater weight for more recent gradients). In step 5, if we ignore ε and steps 3 and 4 (which are technical details anyway), Adam scales down the parameter updates by the square root of **s**. In short, Adam scales down the parameter updates by the ℓ_2 norm of the time-decayed gradients (recall that the ℓ_2 norm is the square root of the sum of squares). AdaMax, introduced in the same paper as Adam, replaces the ℓ_2 norm with the ℓ_∞ norm (a fancy way of saying the max). Specifically, it replaces step 2 in Equation 11-9 with $\mathbf{s} \leftarrow \max\left(\beta_2 \mathbf{s},\ \ \text{abs}(\ \boldsymbol{\nabla}_{\boldsymbol{\theta}} J\left(\boldsymbol{\theta}\right))\right)$, it drops step 4, and in step 5 it scales down the gradient updates by a factor of **s**, which is the max of the absolute value of the time-decayed gradients. In practice, this can make

AdaMax more stable than Adam, but it really depends on the dataset, and in general Adam performs better. So, this is just one more optimizer you can try if you experience problems with Adam on some task.

Nadam

Nadam optimization is Adam optimization plus the Nesterov trick, so it will often converge slightly faster than Adam. In his report introducing this technique,[21] the researcher Timothy Dozat compares many different optimizers on various tasks and finds that Nadam generally outperforms Adam but is sometimes outperformed by RMSProp.

AdamW

AdamW[22] is a variant of Adam that integrates a regularization technique called *weight decay*. Weight decay consists in reducing the size of the model's weights at each training iteration by multiplying them by a decay factor such as 0.99. This may remind you of ℓ_2 regularization (introduced in Chapter 4), which also aims to keep the weights small, and indeed it can be shown mathematically that ℓ_2 regularization is equivalent to weight decay when using SGD. However, when using Adam or its variants, ℓ_2 regularization and weight decay are *not* equivalent: in practice, combining Adam with ℓ_2 regularization results in models that often don't generalize as well as those produced by SGD. AdamW fixes this issue by properly combining Adam with weight decay.

WARNING

Adaptive optimization methods (including RMSProp, Adam, AdaMax, Nadam, and AdamW optimization) are often great, converging fast to a good solution. However, a 2017 paper[23] by Ashia C. Wilson et al. showed that they can lead to solutions that generalize poorly on some datasets. So when you are disappointed by your model's performance, try using Nesterov Accelerated Gradient instead: your dataset may just be allergic to adaptive gradients. Also check out the latest research, because it's moving fast.

To use Nadam or AdaMax in Keras, just use replace `tf.keras.optimizers.Adam` with `tf.keras.optimizers.Nadam` or `tf.keras.optimizers.Adamax`. AdamW is not included in Keras, but it is available in the TensorFlow Add-Ons library. If you followed the installation instructions at *https://homl.info/install* to run everything locally, then you already have this library installed, but if you are using Google Colab, then you need to run `%pip install -q -U tensorflow_addons`. After that, you can use `tfa.optimizers.AdamW` optimizer just like the `tf.keras.optimizers.Adam` optimizer, with an extra `weight_decay` hyperparameter (which needs to be tuned):

```
import tensorflow_addons as tfa

optimizer = tfa.optimizers.AdamW(weight_decay=1e-5,
learning_rate=0.001,
                                 beta_1=0.9, beta_2=0.999)
```

All the optimization techniques discussed so far only rely on the *first-order partial derivatives* (*Jacobians*). The optimization literature also contains amazing algorithms based on the *second-order partial derivatives* (the *Hessians*, which are the partial derivatives of the Jacobians). Unfortunately, these algorithms are very hard to apply to deep neural networks because there are n^2 Hessians per output (where n is the number of parameters), as opposed to just n Jacobians per output. Since DNNs typically have tens of thousands of parameters or more, the second-order optimization algorithms often don't even fit in memory, and even when they do, computing the Hessians is just too slow.

TRAINING SPARSE MODELS

All the optimization algorithms we just discussed produce dense models, meaning that most parameters will be nonzero. If you need a blazingly fast model at runtime, or if you need it to take up less memory, you may prefer to end up with a sparse model instead.

One way to achieve this is to train the model as usual, then get rid of the tiny weights (set them to zero). However, this will typically not lead to a very sparse model, and it may degrade the model's performance.

A better option is to apply strong ℓ_1 regularization during training (we will see how later in this chapter), as it pushes the optimizer to zero out as many weights as it can (as discussed in "Lasso Regression" in Chapter 4).

If these techniques remain insufficient, check out the TensorFlow Model Optimization Toolkit (TF-MOT), which provides a pruning API capable of iteratively removing connections during training based on their magnitude.

Table 11-2 compares all the optimizers we've discussed so far (* is bad, ** is average, and *** is good).

Table 11-2. Optimizer comparison

Class	Convergence speed	Convergence quality

`SGD`	*	***
`SGD(momentum=...)`	**	***
`SGD(momentum=..., nesterov=True)`	**	***
`Adagrad`	***	* (stops too early)
`RMSprop`	***	** or ***
`Adam`	***	** or ***
`AdaMax`	***	** or ***
`Nadam`	***	** or ***
`AdamW`	***	** or ***

Learning Rate Scheduling

Finding a good learning rate is very important. If you set it much too high, training may diverge (as we discussed in "Gradient Descent"). If you set it too low, training will eventually converge to the optimum, but it will take a very long time. If you set it slightly too high, it will make progress very quickly at first, but it will end up dancing around the optimum, never really settling down. If you have a limited computing budget, you may have to interrupt training before it has converged properly, yielding a suboptimal solution (see Figure 11-9).

Figure 11-9. Learning curves for various learning rates η

As we discussed in Chapter 10, you can find a good learning rate by training the model for a few hundred iterations, exponentially increasing the learning rate from a very small value to a very large value, and then looking at the learning curve and picking a learning rate slightly lower than the one at which the learning curve starts shooting back up. You can then reinitialize your model and train it with that learning rate.

But you can do better than a constant learning rate: if you start with a large learning rate and then reduce it once training stops making fast progress, you can reach a good solution faster than with the optimal constant learning rate. There are many different strategies to reduce the learning rate during training. It can also be beneficial to start with a low learning rate, increase it, then drop it again. These strategies are called *learning schedules* (we briefly introduced this concept in Chapter 4). These are the most commonly used learning schedules:

Power scheduling

Set the learning rate to a function of the iteration number t: $\eta(t) = \eta_0 / (1 + t/s)^c$. The initial learning rate η_0, the power c (typically set to 1), and the steps s are hyperparameters. The learning rate drops at each step. After s steps, it is down to $\eta_0 / 2$. After s more steps, it is down to $\eta_0 / 3$, then it goes down to $\eta_0 / 4$, then $\eta_0 / 5$, and so on. As you can see, this schedule first drops quickly, then more and more slowly. Of course, power scheduling requires tuning η_0 and s (and possibly c).

Exponential scheduling

Set the learning rate to $\eta(t) = \eta_0\, 0.1^{t/s}$. The learning rate will gradually drop by a factor of 10 every s steps. While power scheduling reduces the learning rate more and more slowly, exponential scheduling keeps slashing it by a factor of 10 every s steps.

Piecewise constant scheduling

Use a constant learning rate for a number of epochs (e.g., $\eta_0 = 0.1$ for 5 epochs), then a smaller learning rate for another number of epochs (e.g.,

$\eta_1 = 0.001$ for 50 epochs), and so on. Although this solution can work very well, it requires fiddling around to figure out the right sequence of learning rates and how long to use each of them.

Performance scheduling

Measure the validation error every N steps (just like for early stopping), and reduce the learning rate by a factor of λ when the error stops dropping.

1cycle scheduling

1cycle was introduced in a 2018 paper by Leslie Smith.[24] Contrary to the other approaches, it starts by increasing the initial learning rate η_0, growing linearly up to η_1 halfway through training. Then it decreases the learning rate linearly down to η_0 again during the second half of training, finishing the last few epochs by dropping the rate down by several orders of magnitude (still linearly). The maximum learning rate η_1 is chosen using the same approach we used to find the optimal learning rate, and the initial learning rate η_0 is usually 10 times lower. When using a momentum, we start with a high momentum first (e.g., 0.95), then drop it down to a lower momentum during the first half of training (e.g., down to 0.85, linearly), and then bring it back up to the maximum value (e.g., 0.95) during the second half of training, finishing the last few epochs with that maximum value. Smith did many experiments showing that this approach was often able to speed up training considerably and reach better performance. For example, on the popular CIFAR10 image dataset, this approach reached 91.9% validation accuracy in just 100 epochs, instead of 90.3% accuracy in 800 epochs through a standard approach (with the same neural network architecture). This feat was dubbed *super-convergence*.

A 2013 paper by Andrew Senior et al.[25] compared the performance of some of the most popular learning schedules when using momentum optimization to train deep neural networks for speech recognition. The authors concluded that, in this setting, both performance scheduling and exponential scheduling performed well. They favored exponential scheduling because it was easy to tune and it converged slightly faster to the optimal solution. They also mentioned that it was easier to implement than performance scheduling, but in Keras both options are easy. That said, the 1cycle approach seems to perform even better.

Implementing power scheduling in Keras is the easiest option: just set the `decay` hyperparameter when creating an optimizer:

```
optimizer = tf.keras.optimizers.SGD(learning_rate=0.01, decay=1e-4)
```

The `decay` is the inverse of *s* (the number of steps it takes to divide the learning rate by one more unit), and Keras assumes that *c* is equal to 1.

Exponential scheduling and piecewise scheduling are quite simple too. You first need to define a function that takes the current epoch and returns the learning rate. For example, let's implement exponential scheduling:

```
def exponential_decay_fn(epoch):
    return 0.01 * 0.1 ** (epoch / 20)
```

If you do not want to hardcode η_0 and *s*, you can create a function that returns a configured function:

```
def exponential_decay(lr0, s):
    def exponential_decay_fn(epoch):
        return lr0 * 0.1 ** (epoch / s)
    return exponential_decay_fn

exponential_decay_fn = exponential_decay(lr0=0.01, s=20)
```

Next, create a `LearningRateScheduler` callback, giving it the schedule function, and pass this callback to the `fit()` method:

```
lr_scheduler =
tf.keras.callbacks.LearningRateScheduler(exponential_decay_fn)
```

```
history = model.fit(X_train, y_train, [...], callbacks=
[lr_scheduler])
```

The `LearningRateScheduler` will update the optimizer's `learning_rate` attribute at the beginning of each epoch. Updating the learning rate once per epoch is usually enough, but if you want it to be updated more often, for example at every step, you can always write your own callback (see the "Exponential Scheduling" section of the notebook for an example). Updating the learning rate at every step may help if there are many steps per epoch. Alternatively, you can use the `tf.keras.optimizers.schedules` approach, described shortly.

> **TIP**
>
> After training, `history.history["lr"]` gives you access to the list of learning rates used during training.

The schedule function can optionally take the current learning rate as a second argument. For example, the following schedule function multiplies the previous learning rate by $0.1^{1/20}$, which results in the same exponential decay (except the decay now starts at the beginning of epoch 0 instead of 1):

```
def exponential_decay_fn(epoch, lr):
    return lr * 0.1 ** (1 / 20)
```

This implementation relies on the optimizer's initial learning rate (contrary to the previous implementation), so make sure to set it appropriately.

When you save a model, the optimizer and its learning rate get saved along with it. This means that with this new schedule function, you could just load a trained model and continue training where it left off, no problem. Things are not so simple if your schedule function uses the `epoch` argument, however: the epoch does not get saved, and it gets reset to 0 every time you call the `fit()` method. If you were to continue training a model where it left off, this could lead to a very large learning rate, which would likely damage your model's weights. One solution is to manually set the `fit()` method's `initial_epoch` argument so the `epoch` starts at the right value.

For piecewise constant scheduling, you can use a schedule function like the following one (as earlier, you can define a more general function if you want; see the "Piecewise Constant Scheduling" section of the notebook for an example), then create a `LearningRateScheduler` callback with this function and pass it to the `fit()` method, just like we did for exponential scheduling:

```
def piecewise_constant_fn(epoch):
    if epoch < 5:
        return 0.01
    elif epoch < 15:
        return 0.005
    else:
        return 0.001
```

For performance scheduling, use the `ReduceLROnPlateau` callback. For example, if you pass the following callback to the `fit()` method, it will multiply the learning rate by 0.5 whenever the best validation loss does not improve for five consecutive epochs (other options are available; please check the documentation for more details):

```
lr_scheduler = tf.keras.callbacks.ReduceLROnPlateau(factor=0.5,
patience=5)
history = model.fit(X_train, y_train, [...], callbacks=
[lr_scheduler])
```

Lastly, Keras offers an alternative way to implement learning rate scheduling: you can define a scheduled learning rate using one of the classes available in `tf.keras.optimizers.schedules`, then pass it to any optimizer. This approach updates the learning rate at each step rather than at each epoch. For example, here is how to implement the same exponential schedule as the `exponential_decay_fn()` function we defined earlier:

```
import math

batch_size = 32
n_epochs = 25
n_steps = n_epochs * math.ceil(len(X_train) / batch_size)
scheduled_learning_rate =
tf.keras.optimizers.schedules.ExponentialDecay(
    initial_learning_rate=0.01, decay_steps=n_steps,
decay_rate=0.1)
optimizer =
tf.keras.optimizers.SGD(learning_rate=scheduled_learning_rate)
```

This is nice and simple, plus when you save the model, the learning rate and its schedule (including its state) get saved as well.

As for 1cycle, Keras does not support it, but it's possible to implement it in less than 30 lines of code by creating a custom callback that modifies the learning rate at each iteration. To update the optimizer's learning rate from within the callback's `on_batch_begin()` method, you need to call `tf.keras.backend.set_value(self.model.optimizer.learning_rate, new_learning_rate)`. See the "1Cycle scheduling" section of the notebook for an example.

To sum up, exponential decay, performance scheduling, and 1cycle can considerably speed up convergence, so give them a try!

Avoiding Overfitting Through Regularization

> *With four parameters I can fit an elephant and with five I can make him wiggle his trunk.*
>
> —John von Neumann, cited by Enrico Fermi in *Nature* 427

With thousands of parameters, you can fit the whole zoo. Deep neural networks typically have tens of thousands of parameters, sometimes even millions. This gives them an incredible amount of freedom and means they can fit a huge variety of complex datasets. But this great flexibility also makes the network prone to overfitting the training set. Regularization is often needed to prevent this.

We already implemented one of the best regularization techniques in Chapter 10: early stopping. Moreover, even though Batch Normalization was designed to solve the unstable gradients problems, it also acts like a pretty good regularizer. In this section we will examine other popular regularization techniques for neural networks: ℓ_1 and ℓ_2 regularization, dropout, and max-norm regularization.

ℓ_1 and ℓ_2 Regularization

Just like you did in Chapter 4 for simple linear models, you can use ℓ_2 regularization to constrain a neural network's connection weights, and/or ℓ_1 regularization if you want a sparse model (with many weights equal to 0). Here is how to apply ℓ_2 regularization to a Keras layer's connection weights, using a regularization factor of 0.01:

```
layer = tf.keras.layers.Dense(100, activation="relu",
                              kernel_initializer="he_normal",

kernel_regularizer=tf.keras.regularizers.l2(0.01))
```

The `l2()` function returns a regularizer that will be called at each step during training to compute the regularization loss. This is then added to the final loss. As you might expect, you can just use `tf.keras.regularizers.l1()` if you want ℓ_1 regularization; if you want both ℓ_1 and ℓ_2 regularization, use `tf.keras.regularizers.l1_l2()` (specifying both regularization factors).

Since you will typically want to apply the same regularizer to all layers in your network, as well as using the same activation function and the same initialization strategy in all hidden layers, you may find yourself repeating the same arguments. This makes the code ugly and error-prone. To avoid this, you can try refactoring your code to use loops. Another option is to use Python's `functools.partial()` function, which lets you create a thin wrapper for any callable, with some default argument values:

```
from functools import partial

RegularizedDense = partial(tf.keras.layers.Dense,
                           activation="relu",
                           kernel_initializer="he_normal",

kernel_regularizer=tf.keras.regularizers.l2(0.01))

model = tf.keras.Sequential([
    tf.keras.layers.Flatten(input_shape=[28, 28]),
    RegularizedDense(100),
    RegularizedDense(100),
    RegularizedDense(10, activation="softmax")
])
```

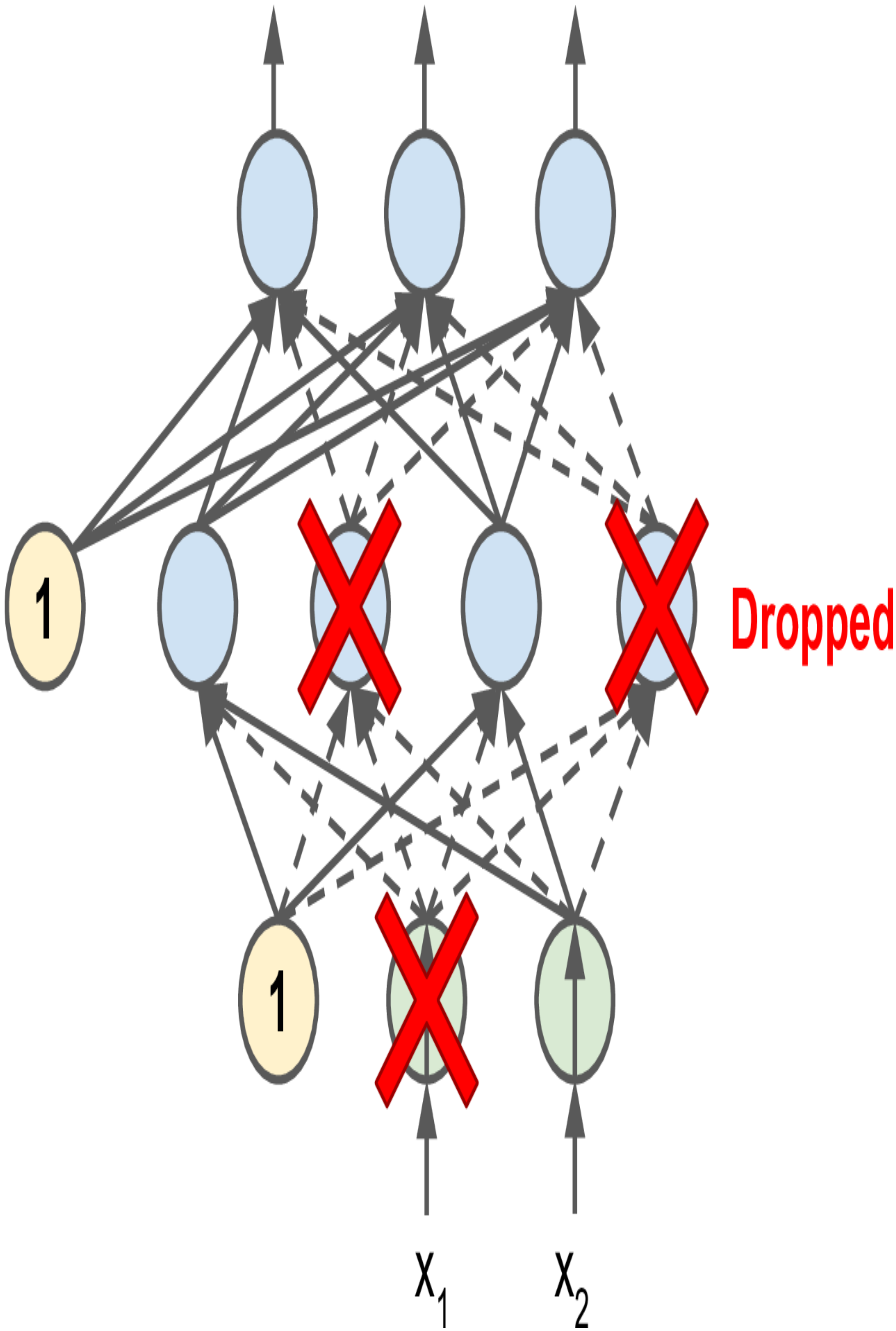
WARNING

As we saw earlier, ℓ_2 regularization is fine when using SGD, momentum optimization and Nesterov momentum optimization, but not with Adam and its variants. If you want to use Adam with weight decay, then do not use ℓ_2 regularization: use AdamW instead.

Dropout

Dropout is one of the most popular regularization techniques for deep neural networks. It was proposed in a paper[26] by Geoffrey Hinton in 2012 and further detailed in a 2014 paper[27] by Nitish Srivastava et al., and it has proven to be highly successful: many state-of-the-art neural networks use dropout, as it gives them a 1–2% accuracy boost. This may not sound like a lot, but when a model already has 95% accuracy, getting a 2% accuracy boost means dropping the error rate by almost 40% (going from 5% error to roughly 3%).

It is a fairly simple algorithm: at every training step, every neuron (including the input neurons, but always excluding the output neurons) has a probability p of being temporarily "dropped out," meaning it will be entirely ignored during this training step, but it may be active during the next step (see Figure 11-10). The hyperparameter *p* is called the *dropout rate*, and it is typically set between 10% and 50%: closer to 20–30% in recurrent neural nets (see Chapter 16), and closer to 40–50% in convolutional neural networks (see Chapter 14). After training, neurons don't get dropped anymore. And that's all (except for a technical detail we will discuss momentarily).



1
Dropped
1
x_1
x_2

Figure 11-10. With dropout regularization, at each training iteration a random subset of all neurons in one or more layers—except the output layer—are "dropped out"; these neurons output 0 at this iteration (represented by the dashed arrows)

It's surprising at first that this destructive technique works at all. Would a company perform better if its employees were told to toss a coin every morning to decide whether or not to go to work? Well, who knows; perhaps it would! The company would be forced to adapt its organization; it could not rely on any single person to work the coffee machine or perform any other critical tasks, so this expertise would have to be spread across several people. Employees would have to learn to cooperate with many of their coworkers, not just a handful of them. The company would become much more resilient. If one person quit, it wouldn't make much of a difference. It's unclear whether this idea would actually work for companies, but it certainly does for neural networks. Neurons trained with dropout cannot co-adapt with their neighboring neurons; they have to be as useful as possible on their own. They also cannot rely excessively on just a few input neurons; they must pay attention to each of their input neurons. They end up being less sensitive to slight changes in the inputs. In the end, you get a more robust network that generalizes better.

Another way to understand the power of dropout is to realize that a unique neural network is generated at each training step. Since each neuron can be either present or absent, there are a total of 2^N possible networks (where N is the total number of droppable neurons). This is such a huge number that it is virtually impossible for the same neural network to be sampled twice. Once you have run 10,000 training steps, you have essentially trained 10,000 different neural networks, each with just one training instance. These neural networks are obviously not independent because they share many of their weights, but they are nevertheless all different. The resulting neural network can be seen as an averaging ensemble of all these smaller neural networks.

TIP

In practice, you can usually apply dropout only to the neurons in the top one to three layers (excluding the output layer).

There is one small but important technical detail. Suppose $p = 75\%$: on average only 25% of all neurons are active at each step during training. This means that after training, a neuron would be connected to four times as many input neurons as it would be during training. To compensate for this fact, we need to multiply each neuron's input connection weights by four during training. If we don't, the neural network will not perform well as it will see different data during and after training. More generally, we need to divide the connection weights by the *keep probability* $(1 – p)$ during training.

To implement dropout using Keras, you can use the `tf.keras.layers.Dropout` layer. During training, it randomly drops some inputs (setting them to 0) and divides the remaining inputs by the keep probability. After training, it does nothing at all; it just passes the inputs to the next layer. The following code applies dropout regularization before every dense layer, using a dropout rate of 0.2:

```
model = tf.keras.Sequential([
    tf.keras.layers.Flatten(input_shape=[28, 28]),
    tf.keras.layers.Dropout(rate=0.2),
    tf.keras.layers.Dense(100, activation="relu",
                          kernel_initializer="he_normal"),
    tf.keras.layers.Dropout(rate=0.2),
    tf.keras.layers.Dense(100, activation="relu",
                          kernel_initializer="he_normal"),
    tf.keras.layers.Dropout(rate=0.2),
    tf.keras.layers.Dense(10, activation="softmax")
])
[...]  # compile and train the model
```

WARNING

Since dropout is only active during training, comparing the training loss and the validation loss can be misleading. In particular, a model may be overfitting the training set and yet have similar training and validation losses. So make sure to evaluate the training loss without dropout (e.g., after training).

If you observe that the model is overfitting, you can increase the dropout rate. Conversely, you should try decreasing the dropout rate if the model underfits the training set. It can also help to increase the dropout rate for large layers, and reduce it for small ones. Moreover, many state-of-the-art architectures only use dropout after the last hidden layer, so you may want to try this if full dropout is too strong.

Dropout does tend to significantly slow down convergence, but it often results in a better model when tuned properly. So, it is generally well worth the extra time and effort, especially for large models.

TIP

If you want to regularize a self-normalizing network based on the SELU activation function (as discussed earlier), you should use *alpha dropout*: this is a variant of dropout that preserves the mean and standard deviation of its inputs. It was introduced in the same paper as SELU, as regular dropout would break self-normalization.

Monte Carlo (MC) Dropout

In 2016, a paper[28] by Yarin Gal and Zoubin Ghahramani added a few more good reasons to use dropout:

- First, the paper established a profound connection between dropout networks (i.e., neural networks containing `Dropout` layers) and approximate Bayesian inference,[29] giving dropout a solid mathematical justification.

- Second, the authors introduced a powerful technique called *MC Dropout*, which can boost the performance of any trained dropout model without having to retrain it or even modify it at all. It also provides a much better measure of the model's uncertainty, and it can be implemented in just a few lines of code.

If this all sounds like some "one weird trick" clickbait, then take a look at the following code. It is the full implementation of *MC Dropout*, boosting the dropout model we trained earlier without retraining it:

```
import numpy as np

y_probas = np.stack([model(X_test, training=True)
                     for sample in range(100)])
y_proba = y_probas.mean(axis=0)
```

Note that `model(X)` is similar to `model.predict(X)` except it returns a tensor rather than a NumPy array, and it supports the `training` argument. In this code example, setting `training=True` ensures that the `Dropout` layer remains active, so all predictions will be a bit different. We just make 100 predictions over the test set, and we compute their average. More specifically, each call to the model returns a matrix with one row per instance and one column per class. Because there are 10,000 instances in the test set and 10 classes, this is a matrix of shape [10000, 10]. We stack 100 such matrices, so `y_probas` is a 3D array of shape [100, 10000, 10]. Once we average over the first dimension (`axis=0`), we get `y_proba`, an array of shape [10000, 10], like we would get with a single prediction. That's all! Averaging over multiple predictions with dropout turned on gives us a Monte Carlo estimate that is generally more reliable than the result of a single prediction with dropout turned off. For example, let's look at the model's prediction for the first instance in the Fashion MNIST test set, with dropout turned off:

```
>>> model.predict(X_test[:1]).round(3)
array([[0.   , 0.   , 0.   , 0.   , 0.   , 0.024, 0.   , 0.132,
0.   ,
        0.844]], dtype=float32)
```

The model is fairly confident (84.4%) that this image belongs to class 9 (ankle boot). Compare this with the MC dropout prediction:

```
>>> y_proba[0].round(3)
array([0.   , 0.   , 0.   , 0.   , 0.   , 0.067, 0.   , 0.209,
0.001,
       0.723], dtype=float32)
```

The model still seems to prefer class 9, but its confidence dropped down to 72.3%, and the estimated probabilities for classes 5 (sandal) and 7 (sneaker) have increased, which makes sense given they're also footwear.

MC Dropout tends to improve the reliability of the model's probability estimates. This means that it's less likely to be confident but wrong, which can be dangerous: just imagine a self-driving car confidently ignoring a stop sign. It's also useful to know exactly which other classes are most likely. And you can also take a look at the standard deviation of the probability estimates:

```
>>> y_std = y_probas.std(axis=0)
>>> y_std[0].round(3)
array([0.   , 0.   , 0.   , 0.001, 0.   , 0.096, 0.   , 0.162,
0.001,
       0.183], dtype=float32)
```

Apparently there's quite a lot of variance in the probability estimates for class 9: the standard deviation is 0.183, which should be compared to the estimated probability of 0.723: if you were building a risk-sensitive system (e.g., a medical or financial system), you would probably treat such an uncertain prediction with extreme caution. You would definitely not treat it like an 84.4% confident prediction. Moreover, the model's accuracy got a (very) small boost from 87.0% to 87.2%:

```
>>> y_pred = y_proba.argmax(axis=1)
>>> accuracy = (y_pred == y_test).sum() / len(y_test)
>>> accuracy
0.8717
```

> **NOTE**
>
> The number of Monte Carlo samples you use (100 in this example) is a hyperparameter you can tweak. The higher it is, the more accurate the predictions and their uncertainty estimates will be. However, if you double it, inference time will also be doubled. Moreover, above a certain number of samples, you will notice little improvement. So your job is to find the right trade-off between latency and accuracy, depending on your application.

If your model contains other layers that behave in a special way during training (such as `BatchNormalization` layers), then you should not force training mode like we just did. Instead, you should replace the `Dropout` layers with the following `MCDropout` class:[30]

```
class MCDropout(tf.keras.layers.Dropout):
    def call(self, inputs, training=None):
        return super().call(inputs, training=True)
```

Here, we just subclass the `Dropout` layer and override the `call()` method to force its `training` argument to `True` (see Chapter 12). Similarly, you could define an `MCAlphaDropout` class by subclassing `AlphaDropout` instead. If you are creating a model from scratch, it's just a matter of using `MCDropout` rather than `Dropout`. But if you have a model that was already trained using `Dropout`, you need to create a new model that's identical to the existing model except with `Dropout` instead of `MCDropout`, then copy the existing model's weights to your new model.

In short, MC Dropout is a great technique that boosts dropout models and provides better uncertainty estimates. And of course, since it is just regular dropout during training, it also acts like a regularizer.

Max-Norm Regularization

Another popular regularization technique for neural networks is called *max-norm regularization*: for each neuron, it constrains the weights **w** of the incoming connections such that $\| \mathbf{w} \|_2 \leq r$, where r is the max-norm hyperparameter and $\| \cdot \|_2$ is the ℓ_2 norm.

Max-norm regularization does not add a regularization loss term to the overall loss function. Instead, it is typically implemented by computing $\| \mathbf{w} \|_2$ after each training step and rescaling $\mathbf{w}$ if needed ($\mathbf{w} \leftarrow \mathbf{w}\, r / \| \mathbf{w} \|_2$).

Reducing r increases the amount of regularization and helps reduce overfitting. Max-norm regularization can also help alleviate the unstable gradients problems (if you are not using Batch Normalization).

To implement max-norm regularization in Keras, set the `kernel_constraint` argument of each hidden layer to a `max_norm()` constraint with the appropriate max value, like this:

```
dense = tf.keras.layers.Dense(
    100, activation="relu", kernel_initializer="he_normal",
    kernel_constraint=tf.keras.constraints.max_norm(1.))
```

After each training iteration, the model's `fit()` method will call the object returned by `max_norm()`, passing it the layer's weights and getting rescaled weights in return, which then replace the layer's weights. As you'll see in Chapter 12, you can define your own custom constraint function if necessary and use it as the `kernel_constraint`. You can also constrain the bias terms by setting the `bias_constraint` argument.

The `max_norm()` function has an `axis` argument that defaults to `0`. A `Dense` layer usually has weights of shape [*number of inputs*, *number of neurons*], so using `axis=0` means that the max-norm constraint will apply independently to each neuron's weight vector. If you want to use max-norm with convolutional layers (see Chapter 14), make sure to set the `max_norm()` constraint's `axis` argument appropriately (usually `axis=[0, 1, 2]`).

Summary and Practical Guidelines

In this chapter we have covered a wide range of techniques, and you may be wondering which ones you should use. This depends on the task, and there is no clear consensus yet, but I have found the configuration in Table 11-3 to work fine in most cases, without requiring much hyperparameter tuning. That said, please do not consider these defaults as hard rules!

Table 11-3. Default DNN configuration

Hyperparameter	Default value

Kernel initializer	He initialization
Activation function	ReLU if shallow; Swish if deep
Normalization	None if shallow; Batch Norm if deep
Regularization	Early stopping; Weight decay if needed
Optimizer	Nesterov Accelerated Gradients or AdamW
Learning rate schedule	Performance scheduling or 1cycle

If the network is a simple stack of dense layers, then it can self-normalize, and you should use the configuration in Table 11-4 instead.

Table 11-4. DNN configuration for a self-n

o
r
m
a
li
z
i
n
g
n
e
t

Hyperparameter	Default value
Kernel initializer	LeCun initialization
Activation function	SELU
Normalization	None (self-normalization)
Regularization	Alpha dropout if needed
Optimizer	Nesterov Accelerated Gradients
Learning rate schedule	Performance scheduling or 1cycle

Don’t forget to normalize the input features! You should also try to reuse parts of a pretrained neural network if you can find one that solves a similar problem, or use unsupervised pretraining if you have a lot of unlabeled data, or use pretraining on an auxiliary task if you have a lot of labeled data for a similar task.

While the previous guidelines should cover most cases, here are some exceptions:

- If you need a sparse model, you can use ℓ_1 regularization (and optionally zero out the tiny weights after training). If you need an even sparser model, you can use the TensorFlow Model Optimization Toolkit. This will break self-normalization, so you should use the default configuration in this case.
- If you need a low-latency model (one that performs lightning-fast predictions), you may need to use fewer layers, use a fast activation function such as ReLU or leaky ReLU, and fold the Batch Normalization layers into the previous layers after training. Having a sparse model will also help. Finally, you may want to reduce the float precision from 32 bits to 16 or even 8 bits (see Chapter 19). Again, check out TF-MOT.
- If you are building a risk-sensitive application, or inference latency is not very important in your application, you can use MC Dropout to boost performance and get more reliable probability estimates, along with uncertainty estimates.

With these guidelines, you are now ready to train very deep nets! I hope you are now convinced that you can go quite a long way using just the convenient Keras API. There may come a time, however, when you need to have even more control; for example, to write a custom loss function or to tweak the training algorithm. For such cases you will need to use TensorFlow's lower-level API, as you will see in the next chapter.

Exercises

1. What is the problem that Glorot initialization and He initialization aim to fix?
2. Is it OK to initialize all the weights to the same value as long as that value is selected randomly using He initialization?
3. Is it OK to initialize the bias terms to 0?

4. In which cases would you want to use each of the activation functions we discussed in this chapter?
5. What may happen if you set the `momentum` hyperparameter too close to 1 (e.g., 0.99999) when using an `SGD` optimizer?
6. Name three ways you can produce a sparse model.
7. Does dropout slow down training? Does it slow down inference (i.e., making predictions on new instances)? What about MC Dropout?
8. Practice training a deep neural network on the CIFAR10 image dataset:

    a. Build a DNN with 20 hidden layers of 100 neurons each (that's too many, but it's the point of this exercise). Use He initialization and the Swish activation function.

    b. Using Nadam optimization and early stopping, train the network on the CIFAR10 dataset. You can load it with `tf.keras.datasets.cifar10.load_data()`. The dataset is composed of 60,000 32 × 32–pixel color images (50,000 for training, 10,000 for testing) with 10 classes, so you'll need a softmax output layer with 10 neurons. Remember to search for the right learning rate each time you change the model's architecture or hyperparameters.

    c. Now try adding Batch Normalization and compare the learning curves: is it converging faster than before? Does it produce a better model? How does it affect training speed?

    d. Try replacing Batch Normalization with SELU, and make the necessary adjustments to ensure the network self-normalizes (i.e., standardize the input features, use LeCun normal initialization, make sure the DNN contains only a sequence of dense layers, etc.).

e. Try regularizing the model with alpha dropout. Then, without retraining your model, see if you can achieve better accuracy using MC Dropout.

f. Retrain your model using 1cycle scheduling and see if it improves training speed and model accuracy.

Solutions to these exercises are available at the end of this chapter's notebook, at *https://homl.info/colab3*.

---

1 Xavier Glorot and Yoshua Bengio, "Understanding the Difficulty of Training Deep Feedforward Neural Networks," *Proceedings of the 13th International Conference on Artificial Intelligence and Statistics* (2010): 249–256.

2 Here's an analogy: if you set a microphone amplifier's knob too close to zero, people won't hear your voice, but if you set it too close to the max, your voice will be saturated and people won't understand what you are saying. Now imagine a chain of such amplifiers: they all need to be set properly in order for your voice to come out loud and clear at the end of the chain. Your voice has to come out of each amplifier at the same amplitude as it came in.

3 E.g., Kaiming He et al., "Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification," *Proceedings of the 2015 IEEE International Conference on Computer Vision* (2015): 1026–1034.

4 A dead neuron may come back to life if its inputs evolve over time and eventually return within a range where the ReLU activation function gets a positive input again. For example, this may happen if Gradient Descent tweaks the neurons in the layers below the dead neuron.

5 Bing Xu et al., "Empirical Evaluation of Rectified Activations in Convolutional Network," arXiv preprint arXiv:1505.00853 (2015).

6 Djork-Arné Clevert et al., "Fast and Accurate Deep Network Learning by Exponential Linear Units (ELUs)," *Proceedings of the International Conference on Learning Representations* (2016).

7 Günter Klambauer et al., "Self-Normalizing Neural Networks," *Proceedings of the 31st International Conference on Neural Information Processing Systems* (2017): 972–981.

8 Dan Hendrycks and Kevin Gimpel, "Gaussian error linear units (GELUs)," arXiv preprint arXiv:1606.08415 (2016).

9 A function is convex if the line segment between any two points on the curve never lies below the curve. A monotonic function only increases, or only decreases.

10 Dan Hendrycks and Kevin Gimpel, “Gaussian error linear units (GELUs),“ arXiv preprint arXiv:1606.08415 (2016).

11 Diganta Misra, “Mish: A self regularized non-monotonic activation function.“ arXiv preprint arXiv:1908.08681 (2019).

12 Sergey Ioffe and Christian Szegedy, “Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift,” *Proceedings of the 32nd International Conference on Machine Learning* (2015): 448–456.

13 However, they are estimated during training, based on the training data, so arguably they *are* trainable. In Keras, “non-trainable” really means “untouched by backpropagation.”

14 Razvan Pascanu et al., “On the Difficulty of Training Recurrent Neural Networks,” *Proceedings of the 30th International Conference on Machine Learning* (2013): 1310–1318.

15 Boris T. Polyak, “Some Methods of Speeding Up the Convergence of Iteration Methods,” *USSR Computational Mathematics and Mathematical Physics* 4, no. 5 (1964): 1–17.

16 Yurii Nesterov, “A Method for Unconstrained Convex Minimization Problem with the Rate of Convergence ټ□/k^2),” *Doklady AN USSR* 269 (1983): 543–547.

17 John Duchi et al., “Adaptive Subgradient Methods for Online Learning and Stochastic Optimization,” *Journal of Machine Learning Research* 12 (2011): 2121–2159.

18 This algorithm was created by Geoffrey Hinton and Tijmen Tieleman in 2012 and presented by Geoffrey Hinton in his Coursera class on neural networks (slides: *https://homl.info/57*; video: *https://homl.info/58*). Amusingly, since the authors did not write a paper to describe the algorithm, researchers often cite “slide 29 in lecture 6e” in their papers.

19 ρis ρletter rho.

20 Diederik P. Kingma and Jimmy Ba, “Adam: A Method for Stochastic Optimization,” arXiv preprint arXiv:1412.6980 (2014).

21 Timothy Dozat, “Incorporating Nesterov Momentum into Adam” (2016).

22 Ilya Loshchilov, and Frank Hutter. “Decoupled weight decay regularization.” arXiv preprint arXiv:1711.05101 (2017).

23 Ashia C. Wilson et al., “The Marginal Value of Adaptive Gradient Methods in Machine Learning,” *Advances in Neural Information Processing Systems* 30 (2017): 4148–4158.

24 Leslie N. Smith, “A Disciplined Approach to Neural Network Hyper-Parameters: Part 1—Learning Rate, Batch Size, Momentum, and Weight Decay,” arXiv preprint arXiv:1803.09820 (2018).

25 Andrew Senior et al., “An Empirical Study of Learning Rates in Deep Neural Networks for Speech Recognition,” *Proceedings of the IEEE International Conference on Acoustics, Speech, and Signal Processing* (2013): 6724–6728.

26 Geoffrey E. Hinton et al., “Improving Neural Networks by Preventing Co-Adaptation of Feature Detectors,” arXiv preprint arXiv:1207.0580 (2012).

27 Nitish Srivastava et al., “Dropout: A Simple Way to Prevent Neural Networks from Overfitting,” *Journal of Machine Learning Research* 15 (2014): 1929–1958.

28 Yarin Gal and Zoubin Ghahramani, “Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning,” *Proceedings of the 33rd International Conference on Machine Learning* (2016): 1050–1059.

29 Specifically, they show that training a dropout network is mathematically equivalent to approximate Bayesian inference in a specific type of probabilistic model called a *Deep Gaussian Process*.

30 This `MCDropout` class will work with all Keras APIs, including the Sequential API. If you only care about the Functional API or the Subclassing API, you do not have to create an `MCDropout` class; you can create a regular `Dropout` layer and call it with `training=True`.

Chapter 12. Custom Models and Training with TensorFlow

A NOTE FOR EARLY RELEASE READERS

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.

This will be the 12th chapter of the final book. Notebooks are available on GitHub at *https://github.com/ageron/handson-ml3*. Datasets are available at *https://github.com/ageron/data*.

If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the editoor at ntache@oreilly.com.

Up until now, we've used only TensorFlow's high-level API, Keras, but it already got us pretty far: we built various neural network architectures, including regression and classification nets, Wide & Deep nets, and self-normalizing nets, using all sorts of techniques, such as Batch Normalization, dropout, and learning rate schedules. In fact, 95% of the use cases you will encounter will not require anything other than Keras (and tf.data; see Chapter 13). But now it's time to dive deeper into TensorFlow and take a look at its lower-level Python API. This will be useful when you need extra control to write custom loss functions, custom metrics, layers, models, initializers, regularizers, weight constraints, and more. You may even need to fully control the training loop itself, for example to apply special transformations or constraints to the gradients (beyond just clipping them) or to use multiple optimizers for different parts of the network. We will cover all these cases in this chapter, and we will also look at how you can boost your custom models and training algorithms using TensorFlow's automatic graph generation feature. But first, let's take a quick tour of TensorFlow.

A Quick Tour of TensorFlow

As you know, TensorFlow is a powerful library for numerical computation, particularly well suited and fine-tuned for large-scale Machine Learning (but you could use it for anything else that requires heavy computations). It was developed by the Google Brain team and it powers many of Google's large-scale services, such as Google Cloud Speech, Google Photos, and Google Search. It was open sourced in November 2015, and it is now the most widely used Deep Learning library in the industry:[1] countless projects use TensorFlow for all sorts of Machine Learning tasks, such as image classification, natural language processing, recommender systems, and time series forecasting.

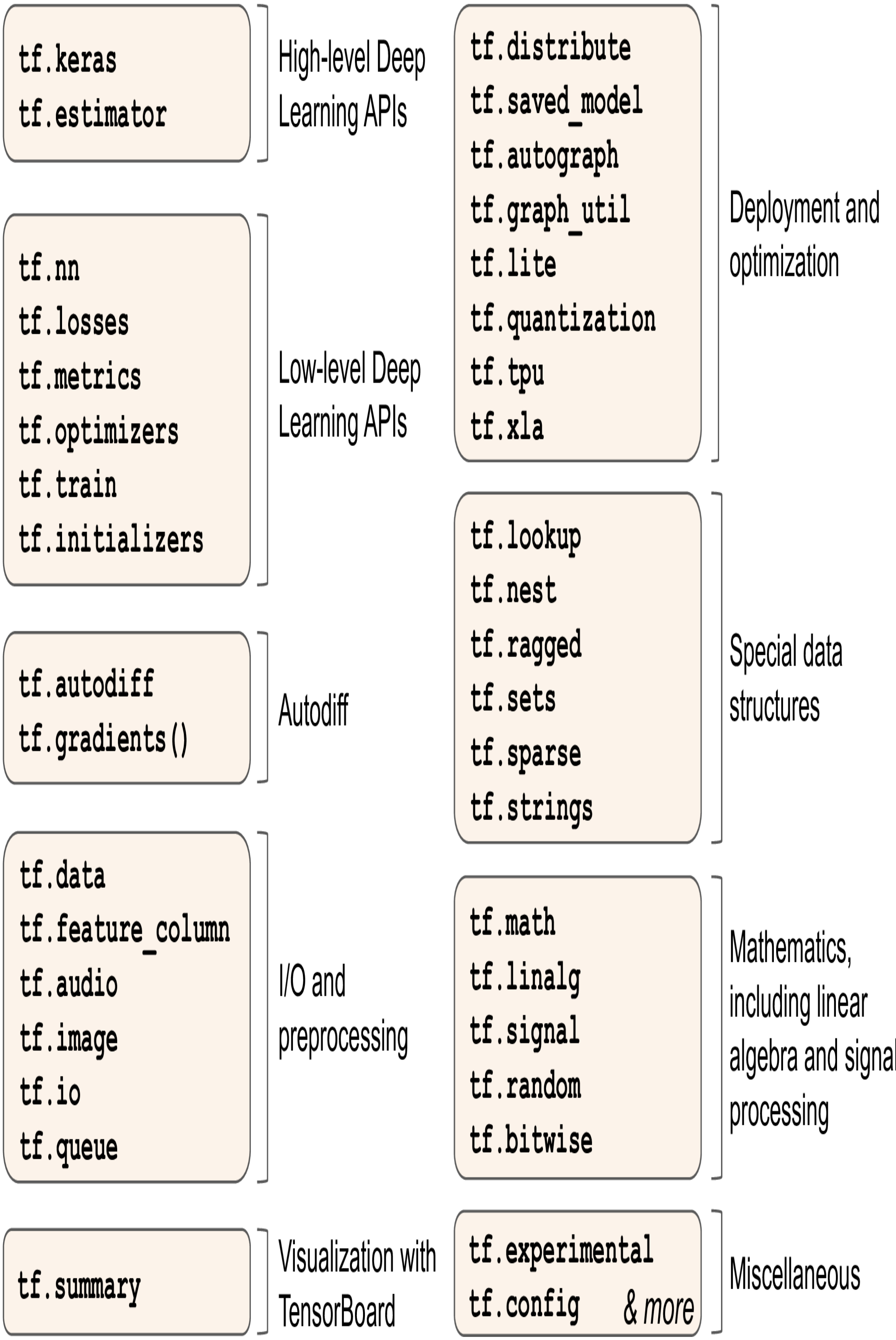
So what does TensorFlow offer? Here's a summary:

- Its core is very similar to NumPy, but with GPU support.
- It supports distributed computing (across multiple devices and servers).
- It includes a kind of just-in-time (JIT) compiler that allows it to optimize computations for speed and memory usage. It works by extracting the *computation graph* from a Python function, then optimizing it (e.g., by pruning unused nodes), and finally running it efficiently (e.g., by automatically running independent operations in parallel).
- Computation graphs can be exported to a portable format, so you can train a TensorFlow model in one environment (e.g., using Python on Linux) and run it in another (e.g., using Java on an Android device).

- It implements reverse-mode autodiff (see Chapter 10 and Appendix B) and provides some excellent optimizers, such as RMSProp and Nadam (see Chapter 11), so you can easily minimize all sorts of loss functions.

TensorFlow offers many more features built on top of these core features: the most important is of course Keras,[2] but it also has data loading and preprocessing ops (`tf.data`, `tf.io`, etc.), image processing ops (`tf.image`), signal processing ops (`tf.signal`), and more (see Figure 12-1 for an overview of TensorFlow's Python API).

> **TIP**
>
> We will cover many of the packages and functions of the TensorFlow API, but it's impossible to cover them all, so you should really take some time to browse through the API; you will find that it is quite rich and well documented.



tf.keras
tf.estimator
High-level Deep Learning APIs
tf.nn
tf.losses
tf.metrics
tf.optimizers
tf.train
tf.initializers
Low-level Deep Learning APIs
tf.autodiff
tf.gradients()
Autodiff
tf.data
tf.feature_column
tf.audio
tf.image
tf.io
tf.queue
I/O and preprocessing
tf.summary
Visualization with TensorBoard
tf.distribute
tf.saved_model
tf.autograph
tf.graph_util
tf.lite
tf.quantization
tf.tpu
tf.xla
Deployment and optimization
tf.lookup
tf.nest
tf.ragged
tf.sets
tf.sparse
tf.strings
Special data structures
tf.math
tf.linalg
tf.signal
tf.random
tf.bitwise
Mathematics, including linear algebra and signal processing
tf.experimental
tf.config
& more
Miscellaneous

Figure 12-1. TensorFlow's Python API

At the lowest level, each TensorFlow operation (*op* for short) is implemented using highly efficient C++ code.[3] Many operations have multiple implementations called *kernels*: each kernel is dedicated to a specific device type, such as CPUs, GPUs, or even TPUs (*tensor processing units*). As you may know, GPUs can dramatically speed up computations by splitting them into many smaller chunks and running them in parallel across many GPU threads. TPUs are even faster: they are custom ASIC chips built specifically for Deep Learning operations[4] (we will discuss how to use TensorFlow with GPUs or TPUs in Chapter 19).

TensorFlow's architecture is shown in Figure 12-2. Most of the time your code will use the high-level APIs (especially Keras and tf.data); but when you need more flexibility, you will use the lower-level Python API, handling tensors directly. Note that APIs for other languages are also available. In any case, TensorFlow's execution engine will take care of running the operations efficiently, even across multiple devices and machines if you tell it to.

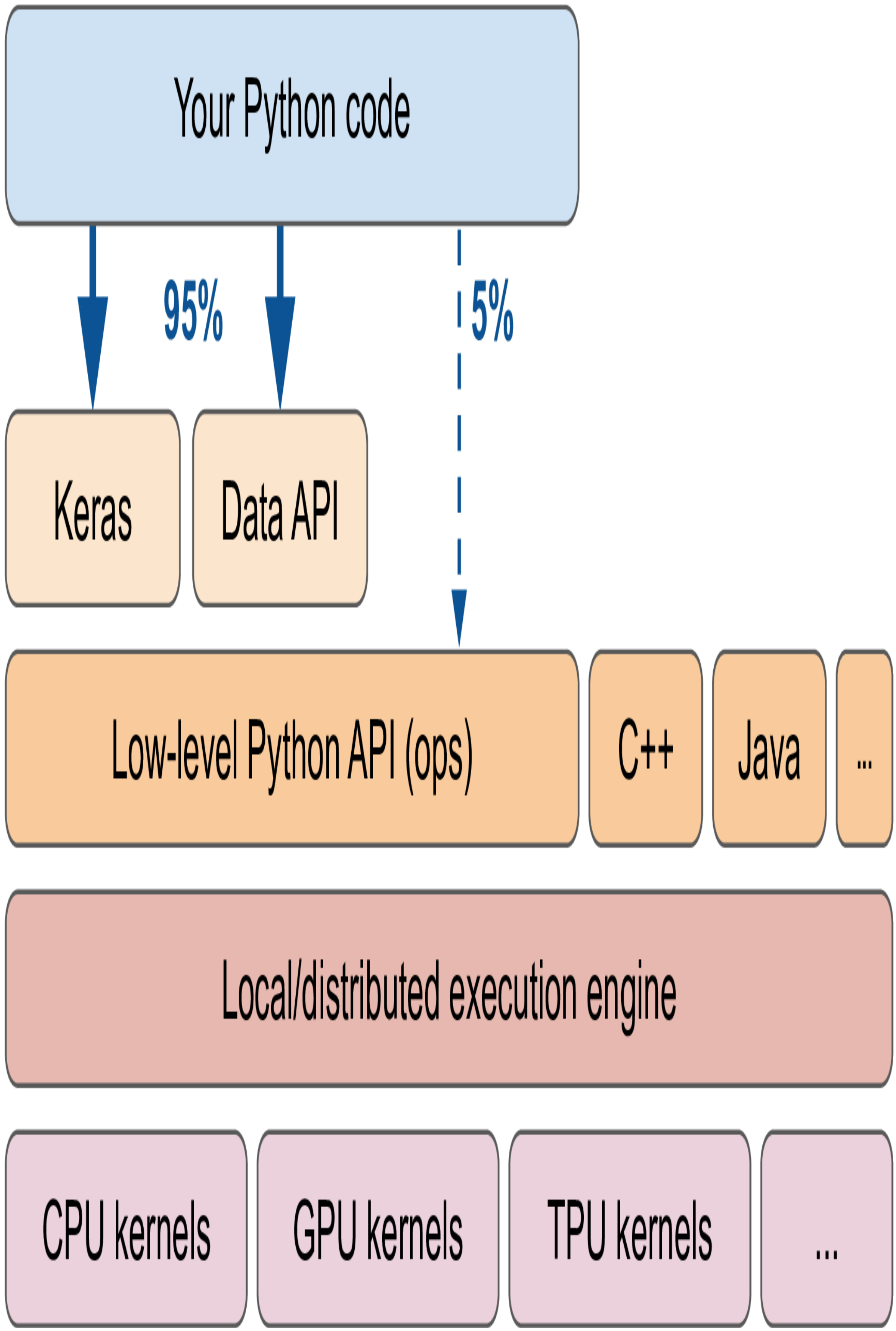

Your Python code
95%
5%
Keras
Data API
Low-level Python API (ops)
C++
Java
...
Local/distributed execution engine
CPU kernels
GPU kernels
TPU kernels
...

Figure 12-2. TensorFlow's architecture

TensorFlow runs not only on Windows, Linux, and macOS, but also on mobile devices (using *TensorFlow Lite*), including both iOS and Android (see Chapter 19). If you do not want to use the Python API, there are C++, Java, and Swift APIs. There is even a JavaScript implementation called *TensorFlow.js* that makes it possible to run your models directly in your browser.

There's more to TensorFlow than the library. TensorFlow is at the center of an extensive ecosystem of libraries. First, there's TensorBoard for visualization (see Chapter 10). Next, there's TensorFlow Extended (TFX), which is a set of libraries built by Google to productionize TensorFlow projects: it includes tools for data validation, preprocessing, model analysis, and serving (with TF Serving; see Chapter 19). Google's *TensorFlow Hub* provides a way to easily download and reuse pretrained neural networks. You can also get many neural network architectures, some of them pretrained, in TensorFlow's model garden. Check out the TensorFlow Resources and *https://github.com/jtoy/awesome-tensorflow* for more TensorFlow-based projects. You will find hundreds of TensorFlow projects on GitHub, so it is often easy to find existing code for whatever you are trying to do.

> **TIP**
>
> More and more ML papers are released along with their implementations, and sometimes even with pretrained models. Check out *https://paperswithcode.com/* to easily find them.

Last but not least, TensorFlow has a dedicated team of passionate and helpful developers, as well as a large community contributing to improving it. To ask technical questions, you should use *http://stackoverflow.com/* and tag your question with *tensorflow* and *python*. You can file bugs and feature requests through GitHub. For general discussions, join the TensorFlow Forum.

OK, it's time to start coding!

Using TensorFlow like NumPy

TensorFlow's API revolves around *tensors*, which flow from operation to operation—hence the name Tensor*Flow*. A tensor is very similar to a NumPy `ndarray`: it is usually a multidimensional array, but it can also hold a scalar (a simple value, such as `42`). These tensors will be important when we create custom cost functions, custom metrics, custom layers, and more, so let's see how to create and manipulate them.

Tensors and Operations

You can create a tensor with `tf.constant()`. For example, here is a tensor representing a matrix with two rows and three columns of floats:

```
>>> import tensorflow as tf
>>> t = tf.constant([[1., 2., 3.], [4., 5., 6.]])  # matrix
>>> t
<tf.Tensor: shape=(2, 3), dtype=float32, numpy=
array([[1., 2., 3.],
       [4., 5., 6.]], dtype=float32)>
```

Just like an `ndarray`, a `tf.Tensor` has a shape and a data type (`dtype`):

```
>>> t.shape
TensorShape([2, 3])
>>> t.dtype
tf.float32
```

Indexing works much like in NumPy:

```
>>> t[:, 1:]
<tf.Tensor: shape=(2, 2), dtype=float32, numpy=
array([[2., 3.],
       [5., 6.]], dtype=float32)>
>>> t[..., 1, tf.newaxis]
```

```
<tf.Tensor: shape=(2, 1), dtype=float32, numpy=
array([[2.],
       [5.]], dtype=float32)>
```

Most importantly, all sorts of tensor operations are available:

```
>>> t + 10
<tf.Tensor: shape=(2, 3), dtype=float32, numpy=
array([[11., 12., 13.],
       [14., 15., 16.]], dtype=float32)>
>>> tf.square(t)
<tf.Tensor: shape=(2, 3), dtype=float32, numpy=
array([[ 1.,  4.,  9.],
       [16., 25., 36.]], dtype=float32)>
>>> t @ tf.transpose(t)
<tf.Tensor: shape=(2, 2), dtype=float32, numpy=
array([[14., 32.],
       [32., 77.]], dtype=float32)>
```

Note that writing `t + 10` is equivalent to calling `tf.add(t, 10)` (indeed, Python calls the magic method `t.__add__(10)`, which just calls `tf.add(t, 10)`). Other operators like `-` and `*` are also supported. The `@` operator was added in Python 3.5, for matrix multiplication: it is equivalent to calling the `tf.matmul()` function.

> **NOTE**
>
> Many functions and classes have aliases. For example, `tf.add()` and `tf.math.add()` are the same function. This allows TensorFlow to have concise names for the most common operations[5] while preserving well-organized packages.

A tensor can also hold a scalar value. In this case, the shape is empty:

```
>>> tf.constant(42)
<tf.Tensor: shape=(), dtype=int32, numpy=42>
```

You will find all the basic math operations you need (`tf.add()`, `tf.multiply()`, `tf.square()`, `tf.exp()`, `tf.sqrt()`, etc.) and most operations that you can find in NumPy (e.g., `tf.reshape()`, `tf.squeeze()`, `tf.tile()`). Some functions have a different name than in NumPy; for instance, `tf.reduce_mean()`, `tf.reduce_sum()`, `tf.reduce_max()`, and `tf.math.log()` are the equivalent of `np.mean()`, `np.sum()`, `np.max()` and `np.log()`. When the name differs, there is usually a good reason for it. For example, in TensorFlow you must write `tf.transpose(t)`; you cannot just write `t.T` like in NumPy. The reason is that the `tf.transpose()` function does not do exactly the same thing as NumPy's `T` attribute: in TensorFlow, a new tensor is created with its own copy of the transposed data, while in NumPy, `t.T` is just a transposed view on the same data. Similarly, the `tf.reduce_sum()` operation is named this way because its GPU kernel (i.e., GPU implementation) uses a reduce algorithm that does not guarantee the order in which the elements are added: because 32-bit floats have limited precision, the result may change ever so slightly every time you call this operation. The same is true of `tf.reduce_mean()` (but of course `tf.reduce_max()` is deterministic).

> **NOTE**
>
> The Keras API has its own low-level API, located in `tf.keras.backend`. This package is usually imported as `K`, for conciseness. It used to include functions like `K.square()`, `K.exp()`, and `K.sqrt()`: this was useful to write portable code back when Keras supported multiple backends, but now that Keras is TensorFlow-only, most of these functions are not needed anymore. Instead, you should call TensorFlow's low-level API directly (e.g., `tf.square()` instead of `K.square()`). Technically `K.square()` and its friends are still there for backward compatibility, but the documentation of the `tf.keras.backend` package only lists a handful of utility functions, such as `clear_session()` (discussed in Chapter 10).

Tensors and NumPy

Tensors play nice with NumPy: you can create a tensor from a NumPy array, and vice versa. You can even apply TensorFlow operations to NumPy arrays and NumPy operations to tensors:

```
>>> import numpy as np
>>> a = np.array([2., 4., 5.])
>>> tf.constant(a)
<tf.Tensor: id=111, shape=(3,), dtype=float64, numpy=array([2.,
4., 5.])>
>>> t.numpy()  # or np.array(t)
array([[1., 2., 3.],
       [4., 5., 6.]], dtype=float32)
>>> tf.square(a)
<tf.Tensor: id=116, shape=(3,), dtype=float64, numpy=array([4.,
16., 25.])>
>>> np.square(t)
array([[ 1.,  4.,  9.],
       [16., 25., 36.]], dtype=float32)
```

WARNING

Notice that NumPy uses 64-bit precision by default, while TensorFlow uses 32-bit. This is because 32-bit precision is generally more than enough for neural networks, plus it runs faster and uses less RAM. So when you create a tensor from a NumPy array, make sure to set `dtype=tf.float32`.

Type Conversions

Type conversions can significantly hurt performance, and they can easily go unnoticed when they are done automatically. To avoid this, TensorFlow does not perform any type conversions automatically: it just raises an exception if you try to execute an operation on tensors with incompatible types. For example, you cannot add a float tensor and an integer tensor, and you cannot even add a 32-bit float and a 64-bit float:

```
>>> tf.constant(2.) + tf.constant(40)
[...] InvalidArgumentError: [...] expected to be a float tensor
[...]
>>> tf.constant(2.) + tf.constant(40., dtype=tf.float64)
[...] InvalidArgumentError: [...] expected to be a float tensor
[...]
```

This may be a bit annoying at first, but remember that it's for a good cause! And of course you can use `tf.cast()` when you really need to convert types:

```
>>> t2 = tf.constant(40., dtype=tf.float64)
>>> tf.constant(2.0) + tf.cast(t2, tf.float32)
<tf.Tensor: id=136, shape=(), dtype=float32, numpy=42.0>
```

Variables

The `tf.Tensor` values we've seen so far are immutable: you cannot modify them. This means that we cannot use regular tensors to implement weights in a neural network, since they need to be tweaked by backpropagation. Plus, other parameters may also need to change over time (e.g., a momentum optimizer keeps track of past gradients). What we need is a `tf.Variable`:

```
>>> v = tf.Variable([[1., 2., 3.], [4., 5., 6.]])
>>> v
<tf.Variable 'Variable:0' shape=(2, 3) dtype=float32, numpy=
array([[1., 2., 3.],
       [4., 5., 6.]], dtype=float32)>
```

A `tf.Variable` acts much like a `tf.Tensor`: you can perform the same operations with it, it plays nicely with NumPy as well, and it is just as picky with types. But it can also be modified in place using the `assign()` method (or `assign_add()` or `assign_sub()`, which increment or decrement the variable by the given value). You can also modify individual cells (or slices), by using the cell's (or slice's) `assign()` method or by using the `scatter_update()` or `scatter_nd_update()` methods:

```
v.assign(2 * v)           # v now equals [[2., 4., 6.], [8., 10.,
12.]]
v[0, 1].assign(42)        # v now equals [[2., 42., 6.], [8.,
10., 12.]]
v[:, 2].assign([0., 1.])  # v now equals [[2., 42., 0.], [8.,
10., 1.]]
v.scatter_nd_update(      # v now equals [[100., 42., 0.], [8.,
10., 200.]]
    indices=[[0, 0], [1, 2]], updates=[100., 200.])
```

Direct assignment will not work:

```
>>> v[1] = [7., 8., 9.]
[...] TypeError: 'ResourceVariable' object does not support item
assignment
```

> **NOTE**
>
> In practice you will rarely have to create variables manually, since Keras provides an `add_weight()` method that will take care of it for you, as we will see. Moreover, model parameters will generally be updated directly by the optimizers, so you will rarely need to update variables manually.

Other Data Structures

TensorFlow supports several other data structures, including the following (please see the "Other Data Structures" section in the notebook or Appendix C for more details):

Sparse tensors (`tf.SparseTensor`)

Efficiently represent tensors containing mostly zeros. The `tf.sparse` package contains operations for sparse tensors.

Tensor arrays (`tf.TensorArray`)

Are lists of tensors. They have a fixed length by default but can optionally be made extensible. All tensors they contain must have the same shape and data type.

Ragged tensors (`tf.RaggedTensor`)

Represent lists of tensors, all of the same rank and data type, but with varying sizes. The dimensions along which the tensor sizes vary are called the *ragged dimensions*. The tf.ragged package contains operations for ragged tensors.

String tensors

Are regular tensors of type `tf.string`. These represent byte strings, not Unicode strings, so if you create a string tensor using a Unicode string (e.g., a regular Python 3 string like `"café"`), then it will get encoded to UTF-8 automatically (e.g., `b"caf\xc3\xa9"`). Alternatively, you can represent Unicode strings using tensors of type `tf.int32`, where each item represents a Unicode code point (e.g., `[99, 97, 102, 233]`). The `tf.strings` package (with an `s`) contains ops for byte strings and Unicode strings (and to convert one into the other). It's important to note that a `tf.string` is atomic, meaning that its length does not appear in the tensor's shape. Once you convert it to a Unicode tensor (i.e., a tensor of type `tf.int32` holding Unicode code points), the length appears in the shape.

Sets

Are represented as regular tensors (or sparse tensors). For example, `tf.constant([[1, 2], [3, 4]])` represents the two sets {1, 2} and {3, 4}. More generally, each set is represented by a vector in the tensor's last axis. You can manipulate sets using operations from the `tf.sets` package.

Queues

Store tensors across multiple steps. TensorFlow offers various kinds of queues: basic First In, First Out (FIFO) queues (`FIFOQueue`), queues that can prioritize some items (`PriorityQueue`), shuffle their items (`RandomShuffleQueue`), and batch items of different shapes by padding (`PaddingFIFOQueue`). These classes are all in the `tf.queue` package.

With tensors, operations, variables, and various data structures at your disposal, you are now ready to customize your models and training algorithms!

Customizing Models and Training Algorithms

Let's start by creating a custom loss function, which is a straightforward and common use case.

Custom Loss Functions

Suppose you want to train a regression model, but your training set is a bit noisy. Of course, you start by trying to clean up your dataset by removing or fixing the outliers, but that turns out to be insufficient; the dataset is still noisy. Which loss function should you use? The mean squared error might penalize large errors too much and cause your model to be imprecise. The mean absolute error would not penalize outliers as much, but training might take a while to converge, and the trained model might not be very precise. This is probably a good time to use the Huber loss (introduced in Chapter 10) instead of the good old MSE. The Huber loss is available in Keras (just use an instance of the `tf.keras.losses.Huber` class). But let's pretend it's not there. To implement it, just create a function that takes the labels and the model's predictions as arguments, and uses TensorFlow operations to compute a tensor containing all the losses (one per sample):

```
def huber_fn(y_true, y_pred):
    error = y_true - y_pred
    is_small_error = tf.abs(error) < 1
    squared_loss = tf.square(error) / 2
    linear_loss  = tf.abs(error) - 0.5
    return tf.where(is_small_error, squared_loss, linear_loss)
```

> **WARNING**
>
> For better performance, you should use a vectorized implementation, as in this example. Moreover, if you want to benefit from TensorFlow's graph optimization features, you should use only TensorFlow operations.

It is also possible to return the mean loss instead of the individual sample losses, but this is not recommended as it makes it impossible to use class weights or sample weights when you need them (see Chapter 10).

Now you can use this Huber loss function when you compile the Keras model, then train your model as usual:

```
model.compile(loss=huber_fn, optimizer="nadam")
model.fit(X_train, y_train, [...])
```

And that's it! For each batch during training, Keras will call the `huber_fn()` function to compute the loss, then it will use reverse-mode autodiff to compute the gradients of the loss with regards to all the model parameters, and finally it will perform a Gradient Descent step (in this example using a Nadam optimizer). Moreover, it will keep track of the total loss since the beginning of the epoch, and it will display the mean loss.

But what happens to this custom loss when you save the model?

Saving and Loading Models That Contain Custom Components

Saving a model containing a custom loss function works fine, but when you load it, you'll need to provide a dictionary that maps the function name to the actual function. More generally, when you load a model containing custom objects, you need to map the names to the objects:

```
model = tf.keras.models.load_model("my_model_with_a_custom_loss",
                                    custom_objects={"huber_fn":
huber_fn})
```

With the current implementation, any error between –1 and 1 is considered "small." But what if you want a different threshold? One solution is to create a function that creates a configured loss function:

```
def create_huber(threshold=1.0):
    def huber_fn(y_true, y_pred):
        error = y_true - y_pred
```

```python
        is_small_error = tf.abs(error) < threshold
        squared_loss = tf.square(error) / 2
        linear_loss  = threshold * tf.abs(error) - threshold ** 2
/ 2
        return tf.where(is_small_error, squared_loss,
linear_loss)
    return huber_fn

model.compile(loss=create_huber(2.0), optimizer="nadam")
```

Unfortunately, when you save the model, the `threshold` will not be saved. This means that you will have to specify the `threshold` value when loading the model (note that the name to use is `"huber_fn"`, which is the name of the function you gave Keras, not the name of the function that created it):

```python
model =
tf.keras.models.load_model("my_model_with_a_custom_loss_threshold
_2.h5",
                                custom_objects={"huber_fn":
create_huber(2.0)})
```

You can solve this by creating a subclass of the `tf.keras.losses.Loss` class, and then implementing its `get_config()` method:

```python
class HuberLoss(tf.keras.losses.Loss):
    def __init__(self, threshold=1.0, **kwargs):
        self.threshold = threshold
        super().__init__(**kwargs)

    def call(self, y_true, y_pred):
        error = y_true - y_pred
        is_small_error = tf.abs(error) < self.threshold
        squared_loss = tf.square(error) / 2
        linear_loss  = self.threshold * tf.abs(error) -
self.threshold**2 / 2
        return tf.where(is_small_error, squared_loss,
linear_loss)

    def get_config(self):
        base_config = super().get_config()
        return {**base_config, "threshold": self.threshold}
```

Let’s walk through this code:

- The constructor accepts `**kwargs` and passes them to the parent constructor, which handles standard hyperparameters: the `name` of the loss and the `reduction` algorithm to use to aggregate the individual instance losses. By default, it is `"AUTO"`, which is equivalent to `"SUM_OVER_BATCH_SIZE"`: the loss will be the sum of the instance losses, weighted by the sample weights, if any, and divided by the batch size (not by the sum of weights, so this is *not* the weighted mean).[6] Other possible values are `"SUM"` and `"NONE"`.

- The `call()` method takes the labels and predictions, computes all the instance losses, and returns them.

- The `get_config()` method returns a dictionary mapping each hyperparameter name to its value. It first calls the parent class’s `get_config()` method, then adds the new hyperparameters to this dictionary.[7]

You can then use any instance of this class when you compile the model:

```
model.compile(loss=HuberLoss(2.), optimizer="nadam")
```

When you save the model, the threshold will be saved along with it; and when you load the model, you just need to map the class name to the class itself:

```
model = 
tf.keras.models.load_model("my_model_with_a_custom_loss_class",
                                      custom_objects={"HuberLoss": 
HuberLoss})
```

When you save a model, Keras calls the loss instance’s `get_config()` method and saves the config in the SavedModel. When you load the model, it calls the `from_config()` class method on the `HuberLoss` class: this method is implemented by the base class (`Loss`) and creates an instance of the class, passing `**config` to the constructor.

That's it for losses! As we will see now, custom activation functions, initializers, regularizers, and constraints are not much different.

Custom Activation Functions, Initializers, Regularizers, and Constraints

Most Keras functionalities, such as losses, regularizers, constraints, initializers, metrics, activation functions, layers, and even full models, can be customized in very much the same way. Most of the time, you will just need to write a simple function with the appropriate inputs and outputs. Here are examples of a custom activation function (equivalent to `tf.keras.activations.softplus()` or `tf.nn.softplus()`), a custom Glorot initializer (equivalent to `tf.keras.initializers.glorot_normal()`), a custom ℓ_1 regularizer (equivalent to `tf.keras.regularizers.l1(0.01)`), and a custom constraint that ensures weights are all positive (equivalent to `tf.keras.constraints.nonneg()` or `tf.nn.relu()`):

```
def my_softplus(z):
    return tf.math.log(1.0 + tf.exp(z))

def my_glorot_initializer(shape, dtype=tf.float32):
    stddev = tf.sqrt(2. / (shape[0] + shape[1]))
    return tf.random.normal(shape, stddev=stddev, dtype=dtype)

def my_l1_regularizer(weights):
    return tf.reduce_sum(tf.abs(0.01 * weights))

def my_positive_weights(weights):  # return value is just
tf.nn.relu(weights)
    return tf.where(weights < 0., tf.zeros_like(weights),
weights)
```

As you can see, the arguments depend on the type of custom function. These custom functions can then be used normally; for example:

```python
layer = tf.keras.layers.Dense(1, activation=my_softplus,

kernel_initializer=my_glorot_initializer,

kernel_regularizer=my_l1_regularizer,

kernel_constraint=my_positive_weights)
```

The activation function will be applied to the output of this `Dense` layer, and its result will be passed on to the next layer. The layer's weights will be initialized using the value returned by the initializer. At each training step the weights will be passed to the regularization function to compute the regularization loss, which will be added to the main loss to get the final loss used for training. Finally, the constraint function will be called after each training step, and the layer's weights will be replaced by the constrained weights.

If a function has hyperparameters that need to be saved along with the model, then you will want to subclass the appropriate class, such as `tf.keras.regularizers.Regularizer`, `tf.keras.constraints.Constraint`, `tf.keras.initializers.Initializer`, or `tf.keras.layers.Layer` (for any layer, including activation functions). Much like we did for the custom loss, here is a simple class for ℓ_1 regularization that saves its `factor` hyperparameter (this time we do not need to call the parent constructor or the `get_config()` method, as they are not defined by the parent class):

```python
class MyL1Regularizer(tf.keras.regularizers.Regularizer):
    def __init__(self, factor):
        self.factor = factor

    def __call__(self, weights):
        return tf.reduce_sum(tf.abs(self.factor * weights))

    def get_config(self):
        return {"factor": self.factor}
```

Note that you must implement the `call()` method for losses, layers (including activation functions), and models, or the `__call__()` method for regularizers, initializers, and constraints. For metrics, things are a bit different, as we will see now.

Custom Metrics

Losses and metrics are conceptually not the same thing: losses (e.g., cross entropy) are used by Gradient Descent to *train* a model, so they must be differentiable (at least at the points where they are evaluated), and their gradients should not be 0 everywhere. Plus, it's OK if they are not easily interpretable by humans. In contrast, metrics (e.g., accuracy) are used to *evaluate* a model: they must be more easily interpretable, and they can be non-differentiable or have 0 gradients everywhere.

That said, in most cases, defining a custom metric function is exactly the same as defining a custom loss function. In fact, we could even use the Huber loss function we created earlier as a metric;[8] it would work just fine (and persistence would also work the same way, in this case only saving the name of the function, `"huber_fn"`, not the threshold):

```
model.compile(loss="mse", optimizer="nadam", metrics=
[create_huber(2.0)])
```

For each batch during training, Keras will compute this metric and keep track of its mean since the beginning of the epoch. Most of the time, this is exactly what you want. But not always! Consider a binary classifier's precision, for example. As we saw in Chapter 3, precision is the number of true positives divided by the number of positive predictions (including both true positives and false positives). Suppose the model made five positive predictions in the first batch, four of which were correct: that's 80% precision. Then suppose the model made three positive predictions in the second batch, but they were all incorrect: that's 0% precision for the second batch. If you just compute the mean of these two precisions, you get 40%. But wait a second—that's *not* the model's precision over these two batches!

Indeed, there were a total of four true positives (4 + 0) out of eight positive predictions (5 + 3), so the overall precision is 50%, not 40%. What we need is an object that can keep track of the number of true positives and the number of false positives and that can compute the precision based on these numbers when requested. This is precisely what the `tf.keras.metrics.Precision` class does:

```
>>> precision = tf.keras.metrics.Precision()
>>> precision([0, 1, 1, 1, 0, 1, 0, 1], [1, 1, 0, 1, 0, 1, 0, 1])
<tf.Tensor: shape=(), dtype=float32, numpy=0.8>
>>> precision([0, 1, 0, 0, 1, 0, 1, 1], [1, 0, 1, 1, 0, 0, 0, 0])
<tf.Tensor: shape=(), dtype=float32, numpy=0.5>
```

In this example, we created a `Precision` object, then we used it like a function, passing it the labels and predictions for the first batch, then for the second batch (you can optionally pass sample weights as well, if you want). We used the same number of true and false positives as in the example we just discussed. After the first batch, it returns a precision of 80%; then after the second batch, it returns 50% (which is the overall precision so far, not the second batch's precision). This is called a *streaming metric* (or *stateful metric*), as it is gradually updated, batch after batch.

At any point, we can call the `result()` method to get the current value of the metric. We can also look at its variables (tracking the number of true and false positives) by using the `variables` attribute, and we can reset these variables using the `reset_states()` method:

```
>>> precision.result()
<tf.Tensor: shape=(), dtype=float32, numpy=0.5>
>>> precision.variables
[<tf.Variable 'true_positives:0' [...], numpy=array([4.],
dtype=float32)>,
 <tf.Variable 'false_positives:0' [...], numpy=array([4.],
dtype=float32)>]
>>> precision.reset_states()  # both variables get reset to 0.0
```

If you need to define your own custom streaming metric, create a subclass of the `tf.keras.metrics.Metric` class. Here is a basic example that keeps track of the total Huber loss and the number of instances seen so far. When asked for the result, it returns the ratio, which is just the mean Huber loss:

```
class HuberMetric(tf.keras.metrics.Metric):
    def __init__(self, threshold=1.0, **kwargs):
        super().__init__(**kwargs)  # handles base args (e.g.,
dtype)
        self.threshold = threshold
        self.huber_fn = create_huber(threshold)
        self.total = self.add_weight("total",
initializer="zeros")
        self.count = self.add_weight("count",
initializer="zeros")

    def update_state(self, y_true, y_pred, sample_weight=None):
        sample_metrics = self.huber_fn(y_true, y_pred)
        self.total.assign_add(tf.reduce_sum(sample_metrics))
        self.count.assign_add(tf.cast(tf.size(y_true),
tf.float32))

    def result(self):
        return self.total / self.count

    def get_config(self):
        base_config = super().get_config()
        return {**base_config, "threshold": self.threshold}
```

Let’s walk through this code:[9]

- The constructor uses the `add_weight()` method to create the variables needed to keep track of the metric’s state over multiple batches—in this case, the sum of all Huber losses (`total`) and the number of instances seen so far (`count`). You could just create variables manually if you preferred. Keras tracks any `tf.Variable` that is set as an attribute (and more generally, any “trackable” object, such as layers or models).

- The `update_state()` method is called when you use an instance of this class as a function (as we did with the `Precision` object). It updates the variables, given the labels and predictions for one batch (and sample weights, but in this case we ignore them).

- The `result()` method computes and returns the final result, in this case the mean Huber metric over all instances. When you use the metric as a function, the `update_state()` method gets called first, then the `result()` method is called, and its output is returned.
- We also implement the `get_config()` method to ensure the `threshold` gets saved along with the model.
- The default implementation of the `reset_states()` method resets all variables to 0.0 (but you can override it if needed).

> **NOTE**
>
> Keras will take care of variable persistence seamlessly; no action is required.

When you define a metric using a simple function, Keras automatically calls it for each batch, and it keeps track of the mean during each epoch, just like we did manually. So the only benefit of our `HuberMetric` class is that the `threshold` will be saved. But of course, some metrics, like precision, cannot simply be averaged over batches: in those cases, there's no other option than to implement a streaming metric.

Now that we have built a streaming metric, building a custom layer will seem like a walk in the park!

Custom Layers

You may occasionally want to build an architecture that contains an exotic layer for which TensorFlow does not provide a default implementation. Or you may simply want to build a very repetitive architecture, in which a particular block of layers is repeated many times, and it would be convenient to treat each block as a single layer. For such cases, you'll want to build a custom layer.

First, some layers have no weights, such as `tf.keras.layers.Flatten` or `tf.keras.layers.ReLU`. If you want to create a custom layer without any weights, the simplest option is to write a function and wrap it in a `tf.keras.layers.Lambda` layer. For example, the following layer will apply the exponential function to its inputs:

```
exponential_layer = tf.keras.layers.Lambda(lambda x: tf.exp(x))
```

This custom layer can then be used like any other layer, using the Sequential API, the Functional API, or the Subclassing API. You can also use it as an activation function, or you could use `activation=tf.exp`. The exponential layer is sometimes used in the output layer of a regression model when the values to predict have very different scales (e.g., 0.001, 10., 1,000.). In fact, the exponential function is one of the standard activation functions in Keras, so you can just use `activation="exponential"`.

As you might guess, to build a custom stateful layer (i.e., a layer with weights), you need to create a subclass of the `tf.keras.layers.Layer` class. For example, the following class implements a simplified version of the `Dense` layer:

```
class MyDense(tf.keras.layers.Layer):
    def __init__(self, units, activation=None, **kwargs):
        super().__init__(**kwargs)
        self.units = units
        self.activation = tf.keras.activations.get(activation)

    def build(self, batch_input_shape):
        self.kernel = self.add_weight(
            name="kernel", shape=[batch_input_shape[-1],
self.units],
            initializer="glorot_normal")
        self.bias = self.add_weight(
            name="bias", shape=[self.units], initializer="zeros")
        super().build(batch_input_shape)  # must be at the end
```

```
    def call(self, X):
        return self.activation(X @ self.kernel + self.bias)

    def compute_output_shape(self, batch_input_shape):
        return tf.TensorShape(batch_input_shape.as_list()[:-1] +
[self.units])

    def get_config(self):
        base_config = super().get_config()
        return {**base_config, "units": self.units,
                "activation":
tf.keras.activations.serialize(self.activation)}
```

Let’s walk through this code:

- The constructor takes all the hyperparameters as arguments (in this example, `units` and `activation`), and importantly it also takes a `**kwargs` argument. It calls the parent constructor, passing it the `kwargs`: this takes care of standard arguments such as `input_shape`, `trainable`, and `name`. Then it saves the hyperparameters as attributes, converting the `activation` argument to the appropriate activation function using the `tf.keras.activations.get()` function (it accepts functions, standard strings like `"relu"` or `"swish"`, or simply `None`).

- The `build()` method’s role is to create the layer’s variables by calling the `add_weight()` method for each weight. The `build()` method is called the first time the layer is used. At that point, Keras will know the shape of this layer’s inputs, and it will pass it to the `build()` method,[10] which is often necessary to create some of the weights. For example, we need to know the number of neurons in the previous layer in order to create the connection weights matrix (i.e., the `"kernel"`): this corresponds to the size of the last dimension of the inputs. At the end of the `build()` method (and only at the end), you must call the parent’s `build()` method: this tells Keras that the layer is built (it just sets `self.built = True`).

- The `call()` method performs the desired operations. In this case, we compute the matrix multiplication of the inputs `X` and the layer's kernel, we add the bias vector, and we apply the activation function to the result, and this gives us the output of the layer.

- The `compute_output_shape()` method simply returns the shape of this layer's outputs. In this case, it is the same shape as the inputs, except the last dimension is replaced with the number of neurons in the layer. Note that in Keras, shapes are instances of the `tf.TensorShape` class, which you can convert to Python lists using `as_list()`.

- The `get_config()` method is just like in the previous custom classes. Note that we save the activation function's full configuration by calling `tf.keras.activations.serialize()`.

You can now use a `MyDense` layer just like any other layer!

> **NOTE**
>
> You can generally omit the `compute_output_shape()` method, as Keras automatically infers the output shape, except when the layer is dynamic (as we will see shortly).

To create a layer with multiple inputs (e.g., `Concatenate`), the argument to the `call()` method should be a tuple containing all the inputs, and similarly the argument to the `compute_output_shape()` method should be a tuple containing each input's batch shape. To create a layer with multiple outputs, the `call()` method should return the list of outputs, and `compute_output_shape()` should return the list of batch output shapes (one per output). For example, the following toy layer takes two inputs and returns three outputs:

```
class MyMultiLayer(tf.keras.layers.Layer):
    def call(self, X):
        X1, X2 = X
        return X1 + X2, X1 * X2, X1 / X2

    def compute_output_shape(self, batch_input_shape):
        batch_input_shape1, batch_input_shape2 =
batch_input_shape
        return [batch_input_shape1, batch_input_shape1,
batch_input_shape1]
```

This layer may now be used like any other layer, but of course only using the Functional and Subclassing APIs, not the Sequential API (which only accepts layers with one input and one output).

If your layer needs to have a different behavior during training and during testing (e.g., if it uses `Dropout` or `BatchNormalization` layers), then you must add a `training` argument to the `call()` method and use this argument to decide what to do. For example, let's create a layer that adds Gaussian noise during training (for regularization) but does nothing during testing (Keras has a layer that does the same thing, `tf.keras.layers.GaussianNoise`):

```
class MyGaussianNoise(tf.keras.layers.Layer):
    def __init__(self, stddev, **kwargs):
        super().__init__(**kwargs)
        self.stddev = stddev

    def call(self, X, training=None):
        if training:
            noise = tf.random.normal(tf.shape(X),
stddev=self.stddev)
            return X + noise
        else:
            return X

    def compute_output_shape(self, batch_input_shape):
        return batch_input_shape
```

With that, you can now build any custom layer you need! Now let's create custom models.

Custom Models

We already looked at creating custom model classes in Chapter 10, when we discussed the Subclassing API.[11] It's straightforward: subclass the `tf.keras.Model` class, create layers and variables in the constructor, and implement the `call()` method to do whatever you want the model to do. For example, suppose you want to build the model represented in Figure 12-3.

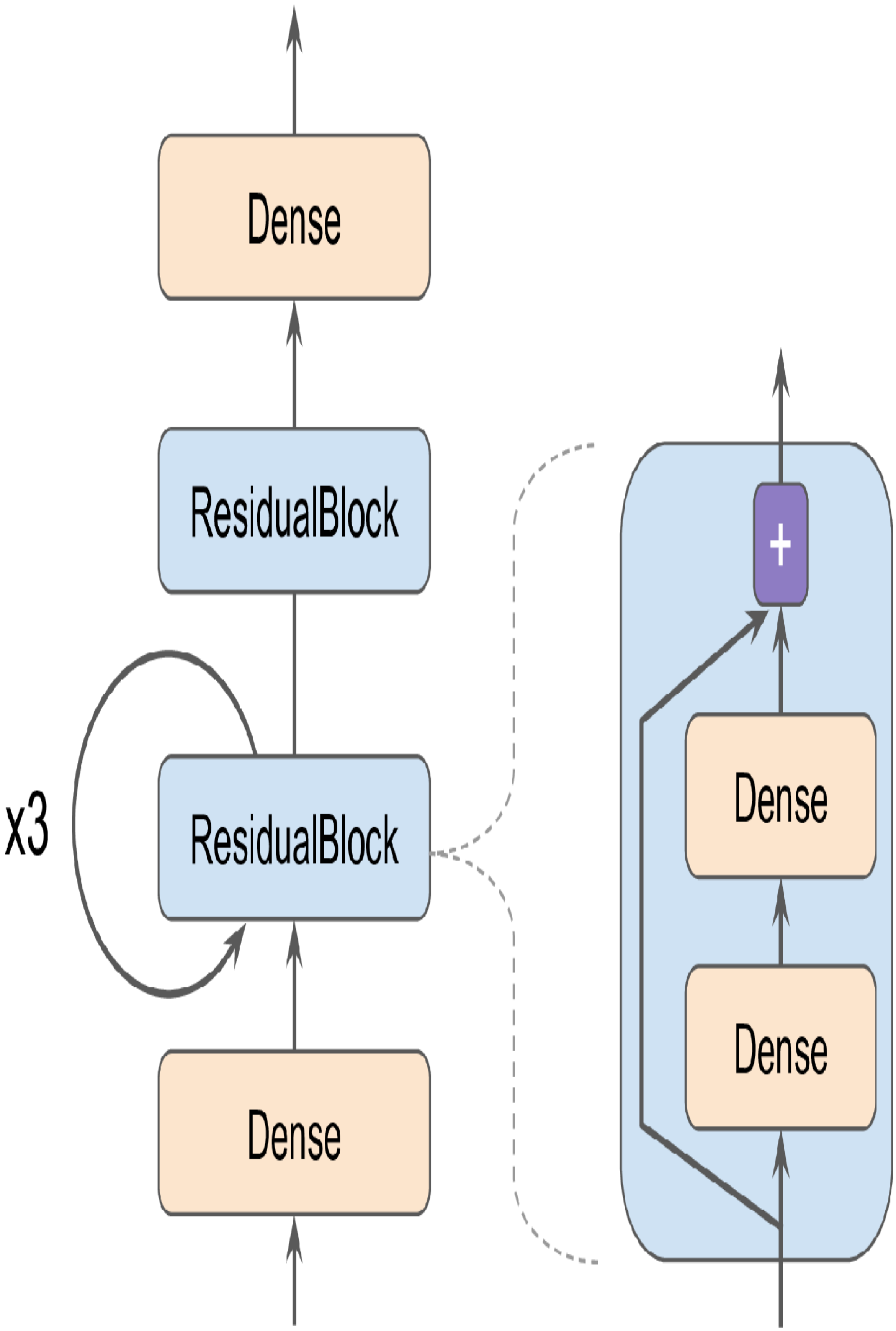

Dense
ResidualBlock
x3
ResidualBlock
Dense
+
Dense
Dense

Figure 12-3. Custom model example: an arbitrary model with a custom ResidualBlock layer containing a skip connection

The inputs go through a first dense layer, then through a *residual block* composed of two dense layers and an addition operation (as we will see in Chapter 14, a residual block adds its inputs to its outputs), then through this same residual block three more times, then through a second residual block, and the final result goes through a dense output layer. Note that this model does not make much sense; it's just an example to illustrate the fact that you can easily build any kind of model you want, even one that contains loops and skip connections. To implement this model, it is best to first create a `ResidualBlock` layer, since we are going to create a couple of identical blocks (and we might want to reuse it in another model):

```
class ResidualBlock(tf.keras.layers.Layer):
    def __init__(self, n_layers, n_neurons, **kwargs):
        super().__init__(**kwargs)
        self.hidden = [tf.keras.layers.Dense(n_neurons,
activation="relu",

kernel_initializer="he_normal")
                       for _ in range(n_layers)]

    def call(self, inputs):
        Z = inputs
        for layer in self.hidden:
            Z = layer(Z)
        return inputs + Z
```

This layer is a bit special since it contains other layers. This is handled transparently by Keras: it automatically detects that the `hidden` attribute contains trackable objects (layers in this case), so their variables are automatically added to this layer's list of variables. The rest of this class is self-explanatory. Next, let's use the Subclassing API to define the model itself:

```
class ResidualRegressor(tf.keras.Model):
    def __init__(self, output_dim, **kwargs):
        super().__init__(**kwargs)
        self.hidden1 = tf.keras.layers.Dense(30,
```

```
activation="relu",

kernel_initializer="he_normal")
        self.block1 = ResidualBlock(2, 30)
        self.block2 = ResidualBlock(2, 30)
        self.out = tf.keras.layers.Dense(output_dim)

    def call(self, inputs):
        Z = self.hidden1(inputs)
        for _ in range(1 + 3):
            Z = self.block1(Z)
        Z = self.block2(Z)
        return self.out(Z)
```

We create the layers in the constructor and use them in the `call()` method. This model can then be used like any other model (compile it, fit it, evaluate it, and use it to make predictions). If you also want to be able to save the model using the `save()` method and load it using the `tf.keras.models.load_model()` function, you must implement the `get_config()` method (as we did earlier) in both the `ResidualBlock` class and the `ResidualRegressor` class. Alternatively, you can save and load the weights using the `save_weights()` and `load_weights()` methods.

The `Model` class is a subclass of the `Layer` class, so models can be defined and used exactly like layers. But a model has some extra functionalities, including of course its `compile()`, `fit()`, `evaluate()`, and `predict()` methods (and a few variants), plus the `get_layers()` method (which can return any of the model's layers by name or by index) and the `save()` method (and support for `tf.keras.models.load_model()` and `tf.keras.models.clone_model()`).

> **TIP**
>
> If models provide more functionality than layers, why not just define every layer as a model? Well, technically you could, but it is usually cleaner to distinguish the internal components of your model (i.e., layers or reusable blocks of layers) from the model itself (i.e., the object you will train). The former should subclass the `Layer` class, while the latter should subclass the `Model` class.

With that, you can naturally and concisely build almost any model that you find in a paper, using the Sequential API, the Functional API, the Subclassing API, or even a mix of these. “Almost” any model? Yes, there are still a few things that we need to look at: first, how to define losses or metrics based on model internals, and second, how to build a custom training loop.

Losses and Metrics Based on Model Internals

The custom losses and metrics we defined earlier were all based on the labels and the predictions (and optionally sample weights). There will be times when you want to define losses based on other parts of your model, such as the weights or activations of its hidden layers. This may be useful for regularization purposes or to monitor some internal aspect of your model.

To define a custom loss based on model internals, compute it based on any part of the model you want, then pass the result to the `add_loss()` method. For example, let’s build a custom regression MLP model composed of a stack of five hidden layers plus an output layer. This custom model will also have an auxiliary output on top of the upper hidden layer. The loss associated to this auxiliary output will be called the *reconstruction loss* (see Chapter 17): it is the mean squared difference between the reconstruction and the inputs. By adding this reconstruction loss to the main loss, we will encourage the model to preserve as much information as possible through the hidden layers—even information that is not directly useful for the regression task itself. In practice, this loss sometimes improves generalization (it is a regularization loss). It is also possible to add a custom metric using the model's `add_metric()` method. Here is the code for this custom model with a custom reconstruction loss and a corresponding metric:

```
class ReconstructingRegressor(tf.keras.Model):
    def __init__(self, output_dim, **kwargs):
        super().__init__(**kwargs)
        self.hidden = [tf.keras.layers.Dense(30,
activation="relu",

kernel_initializer="he_normal")
                       for _ in range(5)]
        self.out = tf.keras.layers.Dense(output_dim)
        self.reconstruction_mean = tf.keras.metrics.Mean(
            name="reconstruction_error")

    def build(self, batch_input_shape):
        n_inputs = batch_input_shape[-1]
        self.reconstruct = tf.keras.layers.Dense(n_inputs)
        super().build(batch_input_shape)  # or self.built = True,
see below

    def call(self, inputs, training=None):
        Z = inputs
        for layer in self.hidden:
            Z = layer(Z)
        reconstruction = self.reconstruct(Z)
        recon_loss = tf.reduce_mean(tf.square(reconstruction -
inputs))
        self.add_loss(0.05 * recon_loss)
        if training:
            result = self.reconstruction_mean(recon_loss)
            self.add_metric(result)
        return self.out(Z)
```

Let's go through this code:

- The constructor creates the DNN with five dense hidden layers and one dense output layer. We also create a `Mean` streaming metric to keep track of the reconstruction error during training.

- The `build()` method creates an extra dense layer which will be used to reconstruct the inputs of the model. It must be created here because its number of units must be equal to the number of inputs, and this number is unknown before the `build()` method is called.[12]

- The `call()` method processes the inputs through all five hidden layers, then passes the result through the reconstruction layer, which produces the reconstruction.

- Then the `call()` method computes the reconstruction loss (the mean squared difference between the reconstruction and the inputs), and adds it to the model's list of losses using the `add_loss()` method.[13] Notice that we scale down the reconstruction loss by multiplying it by 0.05 (this is a hyperparameter you can tune). This ensures that the reconstruction loss does not dominate the main loss.

- Next, during training only, the `call()` method updates the reconstruction metric, and adds it to the model so it can be displayed.

- Finally, the `call()` method passes the output of the hidden layers to the output layer and returns its output.

Both the total loss and the reconstruction loss will go down during training:

```
Epoch 1/5
363/363 [========] - 1s 820us/step - loss: 0.7640 -
reconstruction_error: 1.2728
Epoch 2/5
363/363 [========] - 0s 809us/step - loss: 0.4584 -
reconstruction_error: 0.6340
[...]
```

In most cases, everything we have discussed so far will be sufficient to implement whatever model you want to build, even with complex architectures, losses, and metrics. However, for some architectures such as

GANs (see Chapter 17), you will have to customize the training loop itself. Before we get there, we must look at how to compute gradients automatically in TensorFlow.

Computing Gradients Using Autodiff

To understand how to use autodiff (see Chapter 10 and Appendix B) to compute gradients automatically, let's consider a simple toy function:

```
def f(w1, w2):
    return 3 * w1 ** 2 + 2 * w1 * w2
```

If you know calculus, you can analytically find that the partial derivative of this function with regard to `w1` is `6 * w1` + `2 * w2`. You can also find that its partial derivative with regard to `w2` is `2 * w1`. For example, at the point `(w1, w2)` = `(5, 3)`, these partial derivatives are equal to 36 and 10, respectively, so the gradient vector at this point is (36, 10). But if this were a neural network, the function would be much more complex, typically with tens of thousands of parameters, and finding the partial derivatives analytically by hand would be a virtually impossible task. One solution could be to compute an approximation of each partial derivative by measuring how much the function's output changes when you tweak the corresponding parameter by a tiny amount:

```
>>> w1, w2 = 5, 3
>>> eps = 1e-6
>>> (f(w1 + eps, w2) - f(w1, w2)) / eps
36.000003007075065
>>> (f(w1, w2 + eps) - f(w1, w2)) / eps
10.000000003174137
```

Looks about right! This works rather well and is easy to implement, but it is just an approximation, and importantly you need to call `f()` at least once per parameter (not twice, since we could compute `f(w1, w2)` just once). Having to call `f()` at least once per parameter makes this approach intractable for large neural networks. So instead, we should use reverse-mode autodiff. TensorFlow makes this pretty simple:

```
w1, w2 = tf.Variable(5.), tf.Variable(3.)
with tf.GradientTape() as tape:
    z = f(w1, w2)

gradients = tape.gradient(z, [w1, w2])
```

We first define two variables `w1` and `w2`, then we create a `tf.GradientTape` context that will automatically record every operation that involves a variable, and finally we ask this tape to compute the gradients of the result `z` with regard to both variables `[w1, w2]`. Let's take a look at the gradients that TensorFlow computed:

```
>>> gradients
[<tf.Tensor: shape=(), dtype=float32, numpy=36.0>,
 <tf.Tensor: shape=(), dtype=float32, numpy=10.0>]
```

Perfect! Not only is the result accurate (the precision is only limited by the floating-point errors), but the `gradient()` method only goes through the recorded computations once (in reverse order), no matter how many variables there are, so it is incredibly efficient. It's like magic!

> **TIP**
>
> To save memory, only put the strict minimum inside the `tf.GradientTape()` block. Alternatively, pause recording by creating a `with tape.stop_recording()` block inside the `tf.GradientTape()` block.

The tape is automatically erased immediately after you call its `gradient()` method, so you will get an exception if you try to call `gradient()` twice:

```
with tf.GradientTape() as tape:
    z = f(w1, w2)
```

```
dz_dw1 = tape.gradient(z, w1)  # returns tensor 36.0
dz_dw2 = tape.gradient(z, w2)  # raises a RuntimeError!
```

If you need to call `gradient()` more than once, you must make the tape persistent and delete it each time you are done with it to free resources:[14]

```
with tf.GradientTape(persistent=True) as tape:
    z = f(w1, w2)

dz_dw1 = tape.gradient(z, w1)  # returns tensor 36.0
dz_dw2 = tape.gradient(z, w2)  # returns tensor 10.0, works fine
now!
del tape
```

By default, the tape will only track operations involving variables, so if you try to compute the gradient of `z` with regard to anything other than a variable, the result will be `None`:

```
c1, c2 = tf.constant(5.), tf.constant(3.)
with tf.GradientTape() as tape:
    z = f(c1, c2)

gradients = tape.gradient(z, [c1, c2])  # returns [None, None]
```

However, you can force the tape to watch any tensors you like, to record every operation that involves them. You can then compute gradients with regard to these tensors, as if they were variables:

```
with tf.GradientTape() as tape:
    tape.watch(c1)
    tape.watch(c2)
    z = f(c1, c2)

gradients = tape.gradient(z, [c1, c2])  # returns [tensor 36.,
tensor 10.]
```

This can be useful in some cases, like if you want to implement a regularization loss that penalizes activations that vary a lot when the inputs vary little: the loss will be based on the gradient of the activations with regard to the inputs. Since the inputs are not variables, you would need to tell the tape to watch them.

Most of the time a gradient tape is used to compute the gradients of a single value (usually the loss) with regard to a set of values (usually the model parameters). This is where reverse-mode autodiff shines, as it just needs to do one forward pass and one reverse pass to get all the gradients at once. If you try to compute the gradients of a vector, for example a vector containing multiple losses, then TensorFlow will compute the gradients of the vector's sum. So if you ever need to get the individual gradients (e.g., the gradients of each loss with regard to the model parameters), you must call the tape's `jacobian()` method: it will perform reverse-mode autodiff once for each loss in the vector (all in parallel by default). It is even possible to compute second-order partial derivatives (the Hessians, i.e., the partial derivatives of the partial derivatives), but this is rarely needed in practice (see the "Computing Gradients Using Autodiff" section of the notebook for an example).

In some cases you may want to stop gradients from backpropagating through some part of your neural network. To do this, you must use the `tf.stop_gradient()` function. The function returns its inputs during the forward pass (like `tf.identity()`), but it does not let gradients through during backpropagation (it acts like a constant):

```
def f(w1, w2):
    return 3 * w1 ** 2 + tf.stop_gradient(2 * w1 * w2)

with tf.GradientTape() as tape:
    z = f(w1, w2)  # the forward pass is not affected by
stop_gradient()

gradients = tape.gradient(z, [w1, w2])  # returns [tensor 30.,
None]
```

Finally, you may occasionally run into some numerical issues when computing gradients. For example, if you compute the gradients of the square root function at $x = 10^{-50}$, the result will be infinite. In reality, the slope at that point is not infinite, but it's more than 32-bit floats can handle:

```
>>> x = tf.Variable(1e-50)
>>> with tf.GradientTape() as tape:
...     z = tf.sqrt(x)
...
>>> tape.gradient(z, [x])
[<tf.Tensor: shape=(), dtype=float32, numpy=inf>]
```

To solve this, it's often a good idea to add a tiny value to x (such as 10^{-6}) when computing its square root.

The exponential function is also a frequent source of headaches, as it grows extremely fast. For example, the way `my_softplus()` was defined earlier is not numerically stable. If you compute `my_softplus(100.0)`, you will get infinity rather than the correct result (about 100). But it's possible to rewrite the function to make it numerically stable: the softplus function is defined as $\log(1 + \exp(z))$, which is also equal to $\log(1 + \exp(-|z|)) + \max(z, 0)$ (see the notebook for the mathematical proof) and the advantage of this second form is that the exponential term cannot explode. So here's a better implementation of the `my_softplus()` function:

```
def my_softplus(z):
    return tf.math.log(1 + tf.exp(-tf.abs(z))) + tf.maximum(0.,
z)
```

In some rare cases, a numerically stable function may still have numerically unstable gradients. In such cases, you will have to tell TensorFlow which equation to use for the gradients, rather than letting it use autodiff. For this, you must use the `@tf.custom_gradient` decorator when defining the function, and return both the function's usual result plus a function that computes the gradients. For example, let's update the `my_softplus()` function to also return a numerically stable gradients function:

```
@tf.custom_gradient
def my_softplus(z):
    def my_softplus_gradients(grads):  # grads = backprop'ed from
upper layers
        return grads * (1 - 1 / (1 + tf.exp(z)))  # stable grads
of softplus
```

```
    result = tf.math.log(1 + tf.exp(-tf.abs(z))) + tf.maximum(0.,
z)
    return result, my_softplus_gradients
```

If you know differential calculus (see the tutorial notebook on this topic), you can find that the derivative of log(1 + exp(z)) is exp(z) / (1 + exp(z)). But this form is not stable: for large values of z, it ends up computing infinity divided by infinity, which return NaN. However, with a bit of algebraic manipulation, you can show that it's also equal to 1 - 1 / (1 + exp(z)), which *is* stable. The `my_softplus_gradients()` function uses this equation to compute the gradients. Note that this function will receive as input the gradients that were backpropagated so far, down to the `my_softplus()` function; and according to the chain rule, we must multiply them with this function's gradients.

Now when we compute the gradients of the `my_softplus()` function, we get the proper result, even for large input values.

Congratulations! You can now compute the gradients of any function (provided it is differentiable at the point where you compute it), even blocking backpropagation when needed, and write your own gradient functions! This is probably more flexibility than you will ever need, even if you build your own custom training loops, as we will see now.

Custom Training Loops

In some cases, the `fit()` method may not be flexible enough for what you need to do. For example, the Wide & Deep paper we discussed in Chapter 10 uses two different optimizers: one for the wide path and the other for the deep path. Since the `fit()` method only uses one optimizer (the one that we specify when compiling the model), implementing this paper requires writing your own custom loop.

You may also like to write custom training loops simply to feel more confident that they do precisely what you intend them to do (perhaps you are unsure about some details of the `fit()` method). It can sometimes feel safer to make everything explicit. However, remember that writing a custom training loop will make your code longer, more error-prone, and harder to maintain.

> **TIP**
>
> Unless you're learning or you really need the extra flexibility, you should prefer using the `fit()` method rather than implementing your own training loop, especially if you work in a team.

First, let's build a simple model. No need to compile it, since we will handle the training loop manually:

```
l2_reg = tf.keras.regularizers.l2(0.05)
model = tf.keras.models.Sequential([
    tf.keras.layers.Dense(30, activation="relu",
kernel_initializer="he_normal",
                          kernel_regularizer=l2_reg),
    tf.keras.layers.Dense(1, kernel_regularizer=l2_reg)
])
```

Next, let's create a tiny function that will randomly sample a batch of instances from the training set (in Chapter 13 we will discuss the Data API, which offers a much better alternative):

```
def random_batch(X, y, batch_size=32):
    idx = np.random.randint(len(X), size=batch_size)
    return X[idx], y[idx]
```

Let's also define a function that will display the training status, including the number of steps, the total number of steps, the mean loss since the start of the epoch (i.e., we will use the `Mean` metric to compute it), and other metrics:

```
def print_status_bar(step, total, loss, metrics=None):
    metrics = " - ".join([f"{m.name}: {m.result():.4f}"
                          for m in [loss] + (metrics or [])])
    end = "" if step < total else "\n"
    print(f"\r{step}/{total} - " + metrics, end=end)
```

This code is self-explanatory, unless you are unfamiliar with Python string formatting: `{m.result():.4f}` will format the metric's result as a float with four digits after the decimal point; moreover, using `\r` (carriage return) along with `end=""` ensures that the status bar always gets printed on the same line.

With that, let's get down to business! First, we need to define some hyperparameters and choose the optimizer, the loss function, and the metrics (just the MAE in this example):

```
n_epochs = 5
batch_size = 32
n_steps = len(X_train) // batch_size
optimizer = tf.keras.optimizers.SGD(learning_rate=0.01)
loss_fn = tf.keras.losses.mean_squared_error
mean_loss = tf.keras.metrics.Mean()
metrics = [tf.keras.metrics.MeanAbsoluteError()]
```

And now we are ready to build the custom loop!

```
for epoch in range(1, n_epochs + 1):
    print("Epoch {}/{}".format(epoch, n_epochs))
    for step in range(1, n_steps + 1):
        X_batch, y_batch = random_batch(X_train_scaled, y_train)
        with tf.GradientTape() as tape:
            y_pred = model(X_batch, training=True)
            main_loss = tf.reduce_mean(loss_fn(y_batch, y_pred))
            loss = tf.add_n([main_loss] + model.losses)

        gradients = tape.gradient(loss,
model.trainable_variables)
        optimizer.apply_gradients(zip(gradients,
model.trainable_variables))
        mean_loss(loss)
        for metric in metrics:
            metric(y_batch, y_pred)

        print_status_bar(step, n_steps, mean_loss, metrics)

    for metric in [mean_loss] + metrics:
        metric.reset_states()
```

There’s a lot going on in this code, so let’s walk through it:

- We create two nested loops: one for the epochs, the other for the batches within an epoch.
- Then we sample a random batch from the training set.
- Inside the `tf.GradientTape()` block, we make a prediction for one batch, using the model as a function, and we compute the loss: it is equal to the main loss plus the other losses (in this model, there is one regularization loss per layer). Since the `mean_squared_error()` function returns one loss per instance, we compute the mean over the batch using `tf.reduce_mean()` (if you wanted to apply different weights to each instance, this is where you would do it). The regularization losses are already reduced to a single scalar each, so we just need to sum them (using `tf.add_n()`, which sums multiple tensors of the same shape and data type).
- Next, we ask the tape to compute the gradients of the loss with regard to each trainable variable—*not* all variables!—and we apply them to the optimizer to perform a Gradient Descent step.
- Then we update the mean loss and the metrics (over the current epoch), and we display the status bar.
- At the end of each epoch, we reset the states of the mean loss and the metrics.

If you want to apply Gradient Clipping (see Chapter 11), just set the optimizer’s `clipnorm` or `clipvalue` hyperparameter. If you want to apply any other transformation to the gradients, simply do so before calling the `apply_gradients()` method. And if you want to add weight constraints to your model (e.g., by setting `kernel_constraint` or `bias_constraint` when creating a layer), you should update the training loop to apply these constraints just after `apply_gradients()`, like so:

```
for variable in model.variables:
    if variable.constraint is not None:
        variable.assign(variable.constraint(variable))
```

> **WARNING**
>
> Don't forget to set `training=True` when calling the model in the training loop, especially if your model behaves differently during training and testing (e.g., if it uses `BatchNormalization` or `Dropout`). If it's a custom model, make sure to propagate the `training` argument to the layers that your model calls.

As you can see, there are quite a lot of things you need to get right, and it's easy to make a mistake. But on the bright side, you get full control, so it's your call.

Now that you know how to customize any part of your models[15] and training algorithms, let's see how you can use TensorFlow's automatic graph generation feature: it can speed up your custom code considerably, and it will also make it portable to any platform supported by TensorFlow (see Chapter 19).

TensorFlow Functions and Graphs

Back in TensorFlow 1, graphs were unavoidable (as were the complexities that came with them) because they were a central part of TensorFlow's API. Since TensorFlow 2 (released in 2019), graphs are still there, but not as central, and they're much (much!) simpler to use. To show just how simple, let's start with a trivial function that computes the cube of its input:

```
def cube(x):
    return x ** 3
```

We can obviously call this function with a Python value, such as an int or a float, or we can call it with a tensor:

```
>>> cube(2)
8
>>> cube(tf.constant(2.0))
<tf.Tensor: shape=(), dtype=float32, numpy=8.0>
```

Now, let's use `tf.function()` to convert this Python function to a *TensorFlow Function*:

```
>>> tf_cube = tf.function(cube)
>>> tf_cube
<tensorflow.python.eager.def_function.Function at 0x7fbfe0c54d50>
```

This TF Function can then be used exactly like the original Python function, and it will return the same result (but always as tensors):

```
>>> tf_cube(2)
<tf.Tensor: shape=(), dtype=int32, numpy=8>
>>> tf_cube(tf.constant(2.0))
<tf.Tensor: shape=(), dtype=float32, numpy=8.0>
```

Under the hood, `tf.function()` analyzed the computations performed by the `cube()` function and generated an equivalent computation graph! As you can see, it was rather painless (we will see how this works shortly). Alternatively, we could have used `tf.function` as a decorator; this is actually more common:

```
@tf.function
def tf_cube(x):
    return x ** 3
```

The original Python function is still available via the TF Function's `python_function` attribute, in case you ever need it:

```
>>> tf_cube.python_function(2)
8
```

TensorFlow optimizes the computation graph, pruning unused nodes, simplifying expressions (e.g., 1 + 2 would get replaced with 3), and more.

Once the optimized graph is ready, the TF Function efficiently executes the operations in the graph, in the appropriate order (and in parallel when it can). As a result, a TF Function will usually run much faster than the original Python function, especially if it performs complex computations.[16] Most of the time you will not really need to know more than that: when you want to boost a Python function, just transform it into a TF Function. That's all!

Moreover, when you write a custom loss function, a custom metric, a custom layer, or any other custom function and you use it in a Keras model (as we did throughout this chapter), Keras automatically converts your function into a TF Function—no need to use `tf.function()`. So most of the time, all this magic is 100% transparent.

> **TIP**
>
> You can tell Keras *not* to convert your Python functions to TF Functions by setting `dynamic=True` when creating a custom layer or a custom model. Alternatively, you can set `run_eagerly=True` when calling the model's `compile()` method.

By default, a TF Function generates a new graph for every unique set of input shapes and data types and caches it for subsequent calls. For example, if you call `tf_cube(tf.constant(10))`, a graph will be generated for int32 tensors of shape []. Then if you call `tf_cube(tf.constant(20))`, the same graph will be reused. But if you then call `tf_cube(tf.constant([10, 20]))`, a new graph will be generated for int32 tensors of shape [2]. This is how TF Functions handle polymorphism (i.e., varying argument types and shapes). However, this is only true for tensor arguments: if you pass numerical Python values to a TF Function, a new graph will be generated for every distinct value: for example, calling `tf_cube(10)` and `tf_cube(20)` will generate two graphs.

> **WARNING**
>
> If you call a TF Function many times with different numerical Python values, then many graphs will be generated, slowing down your program and using up a lot of RAM (you must delete the TF Function to release it). Python values should be reserved for arguments that will have few unique values, such as hyperparameters like the number of neurons per layer. This allows TensorFlow to better optimize each variant of your model.

AutoGraph and Tracing

So how does TensorFlow generate graphs? It starts by analyzing the Python function's source code to capture all the control flow statements, such as `for` loops, `while` loops, and `if` statements, as well as `break`, `continue`, and `return` statements. This first step is called *AutoGraph*. The reason TensorFlow has to analyze the source code is that Python does not provide any other way to capture control flow statements: it offers magic methods like `__add__()` and `__mul__()` to capture operators like + and `*`, but there are no `__while__()` or `__if__()` magic methods. After analyzing the function's code, AutoGraph outputs an upgraded version of that function in which all the control flow statements are replaced by the appropriate TensorFlow operations, such as `tf.while_loop()` for loops and `tf.cond()` for `if` statements. For example, in Figure 12-4, AutoGraph analyzes the source code of the `sum_squares()` Python function, and it generates the `tf__sum_squares()` function. In this function, the `for` loop is replaced by the definition of the `loop_body()` function (containing the body of the original `for` loop), followed by a call to the `for_stmt()` function. This call will build the appropriate `tf.while_loop()` operation in the computation graph.

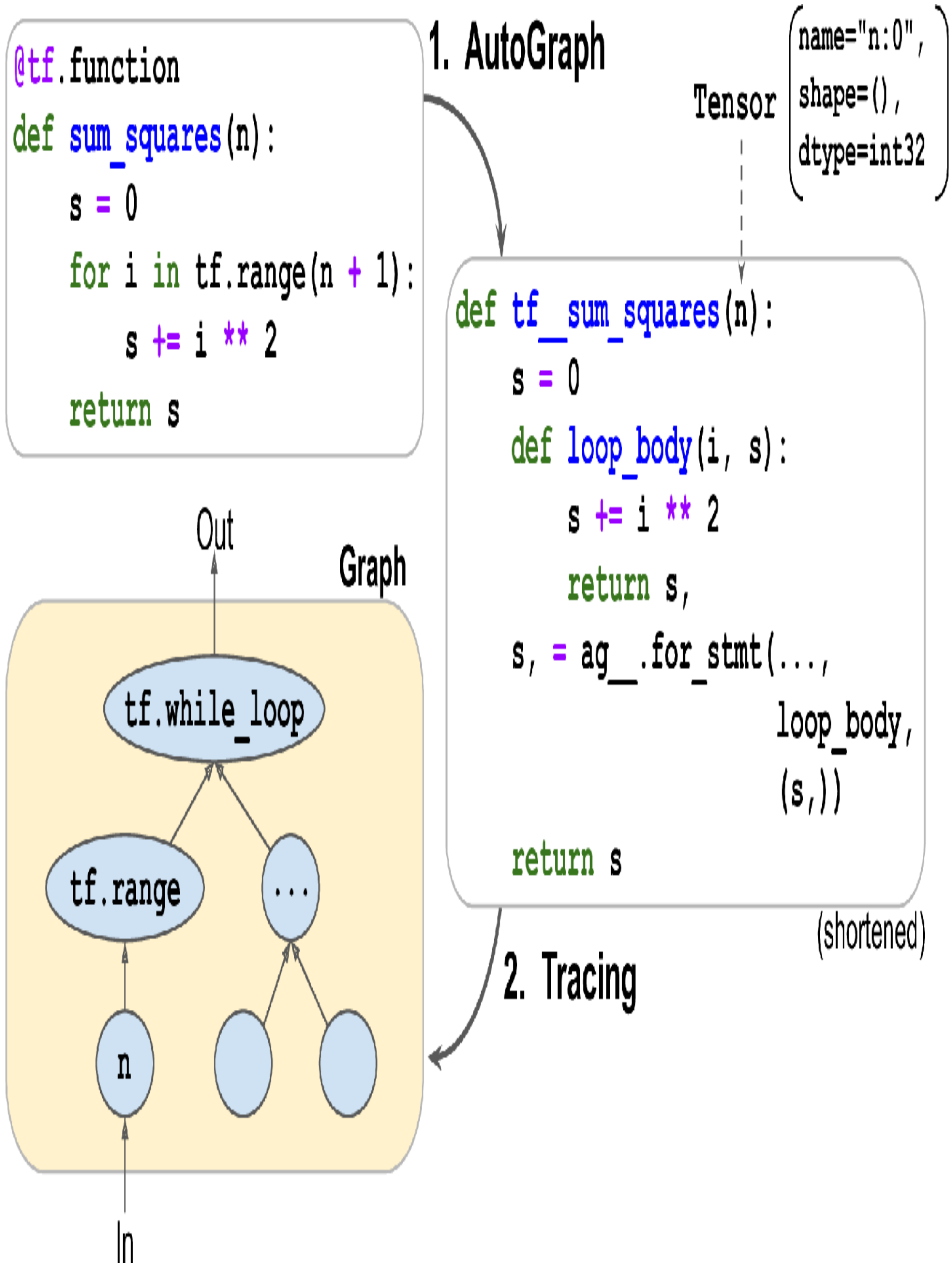


Figure 12-4. How TensorFlow generates graphs using AutoGraph and tracing

Next, TensorFlow calls this “upgraded” function, but instead of passing the argument, it passes a *symbolic tensor*—a tensor without any actual value, only a name, a data type, and a shape. For example, if you call `sum_squares(tf.constant(10))`, then the `tf__sum_squares()` function will be called with a symbolic tensor of type int32 and shape []. The function will run in *graph mode*, meaning that each TensorFlow operation will add a node in the graph to represent itself and its output tensor(s) (as opposed to the regular mode, called *eager execution*, or *eager mode*). In graph mode, TF operations do not perform any computations. Graph mode was the default mode in TensorFlow 1. In Figure 12-4, you can see the `tf__sum_squares()` function being called with a symbolic tensor as its argument (in this case, an int32 tensor of shape []) and the final graph being generated during tracing. The nodes represent operations, and the arrows represent tensors (both the generated function and the graph are simplified).

> **TIP**
>
> To view the generated function’s source code, you can call `tf.autograph.to_code(sum_squares.python_function)`. The code is not meant to be pretty, but it can sometimes help for debugging.

TF Function Rules

Most of the time, converting a Python function that performs TensorFlow operations into a TF Function is trivial: decorate it with `@tf.function` or let Keras take care of it for you. However, there are a few rules to respect:

- If you call any external library, including NumPy or even the standard library, this call will run only during tracing; it will not be part of the graph. Indeed, a TensorFlow graph can only include TensorFlow constructs (tensors, operations, variables, datasets, and so on). So, make sure you use `tf.reduce_sum()` instead of `np.sum()`, `tf.sort()` instead of the built-in `sorted()`

function, and so on (unless you really want the code to run only during tracing). This has a few additional implications:

  - If you define a TF Function `f(x)` that just returns `np.random.rand()`, a random number will only be generated when the function is traced, so `f(tf.constant(2.))` and `f(tf.constant(3.))` will return the same random number, but `f(tf.constant([2., 3.]))` will return a different one. If you replace `np.random.rand()` with `tf.random.uniform([])`, then a new random number will be generated upon every call, since the operation will be part of the graph.

  - If your non-TensorFlow code has side effects (such as logging something or updating a Python counter), then you should not expect those side effects to occur every time you call the TF Function, as they will only occur when the function is traced.

  - You can wrap arbitrary Python code in a `tf.py_function()` operation, but doing so will hinder performance, as TensorFlow will not be able to do any graph optimization on this code. It will also reduce portability, as the graph will only run on platforms where Python is available (and where the right libraries are installed).

- You can call other Python functions or TF Functions, but they should follow the same rules, as TensorFlow will capture their operations in the computation graph. Note that these other functions do not need to be decorated with `@tf.function`.

- If the function creates a TensorFlow variable (or any other stateful TensorFlow object, such as a dataset or a queue), it must do so upon the very first call, and only then, or else you will get an exception. It is usually preferable to create variables outside of the TF Function (e.g., in the `build()` method of a custom layer). If you want to assign a new value to the variable, make sure you call its `assign()` method, instead of using the = operator.

- The source code of your Python function should be available to TensorFlow. If the source code is unavailable (for example, if you define your function in the Python shell, which does not give access to the source code, or if you deploy only the compiled **.pyc* Python files to production), then the graph generation process will fail or have limited functionality.

- TensorFlow will only capture `for` loops that iterate over a tensor or a `tf.data.Dataset` (see Chapter 13). So make sure you use `for i in tf.range(x)` rather than `for i in range(x)`, or else the loop will not be captured in the graph. Instead, it will run during tracing. (This may be what you want if the `for` loop is meant to build the graph, for example to create each layer in a neural network.)

- As always, for performance reasons, you should prefer a vectorized implementation whenever you can, rather than using loops.

It's time to sum up! In this chapter we started with a brief overview of TensorFlow, then we looked at TensorFlow's low-level API, including tensors, operations, variables, and special data structures. We then used these tools to customize almost every component in tf.keras. Finally, we looked at how TF Functions can boost performance, how graphs are generated using AutoGraph and tracing, and what rules to follow when you write TF Functions (if you would like to open the black box a bit further and explore the generated graphs, you will find technical details in Appendix D).

In the next chapter, we will look at how to efficiently load and preprocess data with TensorFlow.

Exercises

1. How would you describe TensorFlow in a short sentence? What are its main features? Can you name other popular Deep Learning libraries?

2. Is TensorFlow a drop-in replacement for NumPy? What are the main differences between the two?

3. Do you get the same result with `tf.range(10)` and `tf.constant(np.arange(10))`?

4. Can you name six other data structures available in TensorFlow, beyond regular tensors?

5. A custom loss function can be defined by writing a function or by subclassing the `tf.keras.losses.Loss` class. When would you use each option?

6. Similarly, a custom metric can be defined in a function or a subclass of `tf.keras.metrics.Metric`. When would you use each option?

7. When should you create a custom layer versus a custom model?

8. What are some use cases that require writing your own custom training loop?

9. Can custom Keras components contain arbitrary Python code, or must they be convertible to TF Functions?

10. What are the main rules to respect if you want a function to be convertible to a TF Function?

11. When would you need to create a dynamic Keras model? How do you do that? Why not make all your models dynamic?

12. Implement a custom layer that performs *Layer Normalization* (we will use this type of layer in Chapter 16):

a. The `build()` method should define two trainable weights **α** and **β**, both of shape `input_shape[-1:]` and data type `tf.float32`. **α** should be initialized with 1s, and **β** with 0s.

b. The `call()` method should compute the mean μ and standard deviation σ of each instance's features. For this, you can use `tf.nn.moments(inputs, axes=-1, keepdims=True)`, which returns the mean μ and the variance σ^2 of all instances (compute the square root of the variance to get the standard deviation). Then the function should compute and return $\boldsymbol{\alpha} \otimes (\mathbf{X} - \mu)/(\sigma + \varepsilon) + \boldsymbol{\beta}$, where $\otimes$ represents itemwise multiplication (`*`) and ε is a smoothing term (small constant to avoid division by zero, e.g., 0.001).

c. Ensure that your custom layer produces the same (or very nearly the same) output as the `tf.keras.layers.LayerNormalization` layer.

13. Train a model using a custom training loop to tackle the Fashion MNIST dataset (see Chapter 10).

    a. Display the epoch, iteration, mean training loss, and mean accuracy over each epoch (updated at each iteration), as well as the validation loss and accuracy at the end of each epoch.

    b. Try using a different optimizer with a different learning rate for the upper layers and the lower layers.

Solutions to these exercises are available at the end of this chapter's notebook, at *https://homl.info/colab3*.

---

1 However, PyTorch is currently more popular in Academia: more papers cite PyTorch than TensorFlow or Keras.

2 TensorFlow includes another Deep Learning API called the *Estimators API*, but the TensorFlow team recommends using Keras instead.

3 If you ever need to (but you probably won't), you can write your own operations using the C++ API.

4 To learn more about TPUs and how they work, check out *https://homl.info/tpus*.

5 A notable exception is `tf.math.log()`, which is commonly used but doesn't have a `tf.log()` alias, as it might be confused with logging.

6 It would not be a good idea to use a weighted mean: if you did, then two instances with the same weight but in different batches would have a different impact on training, depending on the total weight of each batch.

7 The `{**x, [...]}` syntax was added in Python 3.5, to merge all the key/value pairs from dictionary `x` into another dictionary. Since Python 3.9, you can use the nicer `x | y` syntax instead (where `x` and `y` are two dictionaries).

8 However, the Huber loss is seldom used as a metric (the MAE or MSE is preferred).

9 This class is for illustration purposes only. A simpler and better implementation would just subclass the `tf.keras.metrics.Mean` class; see the "Streaming metrics" section of the notebook for an example.

10 The Keras API calls this argument `input_shape`, but since it also includes the batch dimension, I prefer to call it `batch_input_shape`. Same for `compute_output_shape()`.

11 The name "Subclassing API" in Keras usually refers only to the creation of custom models by subclassing, although many other things can be created by subclassing, as we saw in this chapter.

12 Due to TensorFlow issue #46858, the call to `super().build()` may fail in this case, unless the issue was fixed by the time you read this. If not, you need to replace this line with `self.built = True`.

13 You can also call `add_loss()` on any layer inside the model, as the model recursively gathers losses from all of its layers.

14 If the tape goes out of scope, for example when the function that used it returns, Python's garbage collector will delete it for you.

15 With the exception of optimizers, as very few people ever customize these; see the "Custom Optimizers" section in the notebook for an example.

16 However, in this trivial example, the computation graph is so small that there is nothing at all to optimize, so `tf_cube()` actually runs much slower than `cube()`.