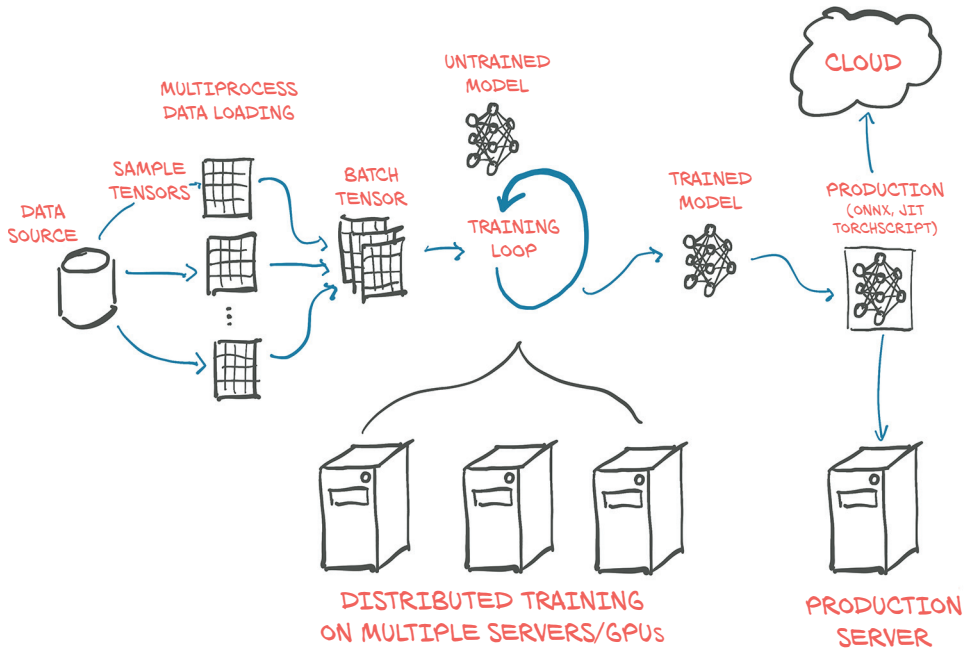
Deep Learning with PyTorch

Eli Stevens
Luca Antiga
Thomas Viehmann

Foreword by Soumith Chintala

MANNING


CLOUD
UNTRAINED MODEL
MULTIPROCESS DATA LOADING
SAMPLE TENSORS
BATCH TENSOR
DATA SOURCE
TRAINING LOOP
TRAINED MODEL
PRODUCTION (ONNX, JIT TORCHSCRIPT)
DISTRIBUTED TRAINING ON MULTIPLE SERVERS/GPUs
PRODUCTION SERVER

Deep Learning with PyTorch

ELI STEVENS, LUCA ANTIGA,
AND THOMAS VIEHMANN
FOREWORD BY SOUMITH CHINTALA

MANNING
SHELTER ISLAND

For online information and ordering of this and other Manning books, please visit www.manning.com. The publisher offers discounts on this book when ordered in quantity. For more information, please contact

Special Sales Department
Manning Publications Co.
20 Baldwin Road
PO Box 761
Shelter Island, NY 11964
Email: orders@manning.com

Manning Publications Co.
20 Baldwin Road
PO Box 761
Shelter Island, NY 11964

Development editor: Frances Lefkowitz
Technical development editor: Arthur Zubarev
Review editor: Ivan Martinović
Production editor: Deirdre Hiam
Copyeditor: Tiffany Taylor
Proofreader: Katie Tennant
Technical proofreader: Kostas Passadis
Typesetter: Gordan Salinovic
Cover designer: Marija Tudor

ISBN 9781617295263
Printed in the United States of America

To my wife (this book would not have happened without her invaluable support and partnership),
my parents (I would not have happened without them),
and my children (this book would have happened a lot sooner but for them).

Thank you for being my home, my foundation, and my joy.
—Eli Stevens

Same :-) But, really, this is for you, Alice and Luigi.
—Luca Antiga

To Eva, Rebekka, Jonathan, and David.
—Thomas Viehmann

contents

foreword

When we started the PyTorch project in mid-2016, we were a band of open source hackers who met online and wanted to write better deep learning software. Two of the three authors of this book, Luca Antiga and Thomas Viehmann, were instrumental in developing PyTorch and making it the success that it is today.

Our goal with PyTorch was to build the most flexible framework possible to express deep learning algorithms. We executed with focus and had a relatively short development time to build a polished product for the developer market. This wouldn't have been possible if we hadn't been standing on the shoulders of giants. PyTorch derives a significant part of its codebase from the Torch7 project started in 2007 by Ronan Collobert and others, which has roots in the Lush programming language pioneered by Yann LeCun and Leon Bottou. This rich history helped us focus on what needed to change, rather than conceptually starting from scratch.

It is hard to attribute the success of PyTorch to a single factor. The project offers a good user experience and enhanced debuggability and flexibility, ultimately making users more productive. The huge adoption of PyTorch has resulted in a beautiful ecosystem of software and research built on top of it, making PyTorch even richer in its experience.

Several courses and university curricula, as well as a huge number of online blogs and tutorials, have been offered to make PyTorch easier to learn. However, we have seen very few books. In 2017, when someone asked me, "When is the PyTorch book going to be written?" I responded, "If it gets written now, I can guarantee that it will be outdated by the time it is completed."

With the publication of *Deep Learning with PyTorch*, we finally have a definitive treatise on PyTorch. It covers the basics and abstractions in great detail, tearing apart the underpinnings of data structures like tensors and neural networks and making sure you understand their implementation. Additionally, it covers advanced subjects such as JIT and deployment to production (an aspect of PyTorch that no other book currently covers).

Additionally, the book covers applications, taking you through the steps of using neural networks to help solve a complex and important medical problem. With Luca's deep expertise in bioengineering and medical imaging, Eli's practical experience creating software for medical devices and detection, and Thomas's background as a PyTorch core developer, this journey is treated carefully, as it should be.

All in all, I hope this book becomes your "extended" reference document and an important part of your library or workshop.

Soumith Chintala
Cocreator of PyTorch

preface

As kids in the 1980s, taking our first steps on our Commodore VIC 20 (Eli), the Sinclair Spectrum 48K (Luca), and the Commodore C16 (Thomas), we saw the dawn of personal computers, learned to code and write algorithms on ever-faster machines, and often dreamed about where computers would take us. We also were painfully aware of the gap between what computers did in movies and what they could do in real life, collectively rolling our eyes when the main character in a spy movie said, "Computer, enhance."

Later on, during our professional lives, two of us, Eli and Luca, independently challenged ourselves with medical image analysis, facing the same kind of struggle when writing algorithms that could handle the natural variability of the human body. There was a lot of heuristics involved when choosing the best mix of algorithms that could make things work and save the day. Thomas studied neural nets and pattern recognition at the turn of the century but went on to get a PhD in mathematics doing modeling.

When deep learning came about at the beginning of the 2010s, making its initial appearance in computer vision, it started being applied to medical image analysis tasks like the identification of structures or lesions on medical images. It was at that time, in the first half of the decade, that deep learning appeared on our individual radars. It took a bit to realize that deep learning represented a whole new way of writing software: a new class of multipurpose algorithms that could learn how to solve complicated tasks through the observation of data.

To our kids-of-the-80s minds, the horizon of what computers could do expanded overnight, limited not by the brains of the best programmers, but by the data, the neural network architecture, and the training process. The next step was getting our hands dirty. Luca choose Torch 7 (http://torch.ch), a venerable precursor to PyTorch; it's nimble, lightweight, and fast, with approachable source code written in Lua and plain C, a supportive community, and a long history behind it. For Luca, it was love at first sight. The only real drawback with Torch 7 was being detached from the ever-growing Python data science ecosystem that the other frameworks could draw from. Eli had been interested in AI since college,[1] but his career pointed him in other directions, and he found other, earlier deep learning frameworks a bit too laborious to get enthusiastic about using them for a hobby project.

So we all got really excited when the first PyTorch release was made public on January 18, 2017. Luca started contributing to the core, and Eli was part of the community very early on, submitting the odd bug fix, feature, or documentation update. Thomas contributed a ton of features and bug fixes to PyTorch and eventually became one of the independent core contributors. There was the feeling that something big was starting up, at the right level of complexity and with a minimal amount of cognitive overhead. The lean design lessons learned from the Torch 7 days were being carried over, but this time with a modern set of features like automatic differentiation, dynamic computation graphs, and NumPy integration.

Given our involvement and enthusiasm, and after organizing a couple of PyTorch workshops, writing a book felt like a natural next step. The goal was to write a book that would have been appealing to our former selves getting started just a few years back.

Predictably, we started with grandiose ideas: teach the basics, walk through end-to-end projects, and demonstrate the latest and greatest models in PyTorch. We soon realized that would take a lot more than a single book, so we decided to focus on our initial mission: devote time and depth to cover the key concepts underlying PyTorch, assuming little or no prior knowledge of deep learning, and get to the point where we could walk our readers through a complete project. For the latter, we went back to our roots and chose to demonstrate a medical image analysis challenge.

[1] Back when "deep" neural networks meant *three* hidden layers!

acknowledgments

We are deeply indebted to the PyTorch team. It is through their collective effort that PyTorch grew organically from a summer internship project to a world-class deep learning tool. We would like to mention Soumith Chintala and Adam Paszke, who, in addition to their technical excellence, worked actively toward adopting a "community first" approach to managing the project. The level of health and inclusiveness in the PyTorch community is a testament to their actions.

Speaking of community, PyTorch would not be what it is if not for the relentless work of individuals helping early adopters and experts alike on the discussion forum. Of all the honorable contributors, Piotr Bialecki deserves our particular badge of gratitude. Speaking of the book, a particular shout-out goes to Joe Spisak, who believed in the value that this book could bring to the community, and also Jeff Smith, who did an incredible amount of work to bring that value to fruition. Bruce Lin's work to excerpt part 1 of this text and provide it to the PyTorch community free of charge is also hugely appreciated.

We would like to thank the team at Manning for guiding us through this journey, always aware of the delicate balance between family, job, and writing in our respective lives. Thanks to Erin Twohey for reaching out and asking if we'd be interested in writing a book, and thanks to Michael Stephens for tricking us into saying yes. We *told* you we had no time! Brian Hanafee went above and beyond a reviewer's duty. Arthur Zubarev and Kostas Passadis gave great feedback, and Jennifer Houle had to deal with our wacky art style. Our copyeditor, Tiffany Taylor, has an impressive eye for detail; any mistakes are ours and ours alone. We would also like to thank our project editor,

Deirdre Hiam, our proofreader, Katie Tennant, and our review editor, Ivan Martinović. There are also a host of people working behind the scenes, glimpsed only on the CC list of status update threads, and all necessary to bring this book to print. Thank you to every name we've left off this list! The anonymous reviewers who gave their honest feedback helped make this book what it is.

Frances Lefkowitz, our tireless editor, deserves a medal and a week on a tropical island after dragging this book over the finish line. Thank you for all you've done and for the grace with which you did it.

We would also like to thank our reviewers, who have helped to improve our book in many ways: Aleksandr Erofeev, Audrey Carstensen, Bachir Chihani, Carlos Andres Mariscal, Dale Neal, Daniel Berecz, Doniyor Ulmasov, Ezra Stevens, Godfred Asamoah, Helen Mary Labao Barrameda, Hilde Van Gysel, Jason Leonard, Jeff Coggshall, Kostas Passadis, Linnsey Nil, Mathieu Zhang, Michael Constant, Miguel Montalvo, Orlando Alejo Méndez Morales, Philippe Van Bergen, Reece Stevens, Srinivas K. Raman, and Yujan Shrestha.

To our friends and family, wondering what rock we've been hiding under these past two years: Hi! We missed you! Let's have dinner sometime.

about this book

This book has the aim of providing the foundations of deep learning with PyTorch and showing them in action in a real-life project. We strive to provide the key concepts underlying deep learning and show how PyTorch puts them in the hands of practitioners. In the book, we try to provide intuition that will support further exploration, and in doing so we selectively delve into details to show what is going on behind the curtain.

Deep Learning with PyTorch doesn't try to be a reference book; rather, it's a conceptual companion that will allow you to independently explore more advanced material online. As such, we focus on a subset of the features offered by PyTorch. The most notable absence is recurrent neural networks, but the same is true for other parts of the PyTorch API.

Who should read this book

This book is meant for developers who are or aim to become deep learning practitioners and who want to get acquainted with PyTorch. We imagine our typical reader to be a computer scientist, data scientist, or software engineer, or an undergraduate-or-later student in a related program. Since we don't assume prior knowledge of deep learning, some parts in the first half of the book may be a repetition of concepts that are already known to experienced practitioners. For those readers, we hope the exposition will provide a slightly different angle to known topics.

We expect readers to have basic knowledge of imperative and object-oriented programming. Since the book uses Python, you should be familiar with the syntax and operating environment. Knowing how to install Python packages and run scripts on

your platform of choice is a prerequisite. Readers coming from C++, Java, JavaScript, Ruby, or other such languages should have an easy time picking it up but will need to do some catch-up outside this book. Similarly, being familiar with NumPy will be useful, if not strictly required. We also expect familiarity with some basic linear algebra, such as knowing what matrices and vectors are and what a dot product is.

How this book is organized: A roadmap

Deep Learning with PyTorch is organized in three distinct parts. Part 1 covers the foundations, while part 2 walks you through an end-to-end project, building on the basic concepts introduced in part 1 and adding more advanced ones. The short part 3 rounds off the book with a tour of what PyTorch offers for deployment. You will likely notice different voices and graphical styles among the parts. Although the book is a result of endless hours of collaborative planning, discussion, and editing, the act of writing and authoring graphics was split among the parts: Luca was primarily in charge of part 1 and Eli of part 2.[2] When Thomas came along, he tried to blend the style in part 3 and various sections here and there with the writing in parts 1 and 2. Rather than finding a minimum common denominator, we decided to preserve the original voices that characterized the parts.

Following is a breakdown of each part into chapters and a brief description of each.

PART 1

In part 1, we take our first steps with PyTorch, building the fundamental skills needed to understand PyTorch projects out there in the wild as well as starting to build our own. We'll cover the PyTorch API and some behind-the-scenes features that make PyTorch the library it is, and work on training an initial classification model. By the end of part 1, we'll be ready to tackle a real-world project.

Chapter 1 introduces PyTorch as a library and its place in the deep learning revolution, and touches on what sets PyTorch apart from other deep learning frameworks.

Chapter 2 shows PyTorch in action by running examples of pretrained networks; it demonstrates how to download and run models in PyTorch Hub.

Chapter 3 introduces the basic building block of PyTorch—the tensor—showing its API and going behind the scenes with some implementation details.

Chapter 4 demonstrates how different kinds of data can be represented as tensors and how deep learning models expects tensors to be shaped.

Chapter 5 walks through the mechanics of learning through gradient descent and how PyTorch enables it with automatic differentiation.

Chapter 6 shows the process of building and training a neural network for regression in PyTorch using the `nn` and `optim` modules.

Chapter 7 builds on the previous chapter to create a fully connected model for image classification and expand the knowledge of the PyTorch API.

Chapter 8 introduces convolutional neural networks and touches on more advanced concepts for building neural network models and their PyTorch implementation.

[2] A smattering of Eli's and Thomas's art appears in other parts; don't be shocked if the style changes mid-chapter!

PART 2

In part 2, each chapter moves us closer to a comprehensive solution to automatic detection of lung cancer. We'll use this difficult problem as motivation to demonstrate the real-world approaches needed to solve large-scale problems like cancer screening. It is a large project with a focus on clean engineering, troubleshooting, and problem solving.

Chapter 9 describes the end-to-end strategy we'll use for lung tumor classification, starting from computed tomography (CT) imaging.

Chapter 10 loads the human annotation data along with the images from CT scans and converts the relevant information into tensors, using standard PyTorch APIs.

Chapter 11 introduces a first classification model that consumes the training data introduced in chapter 10. We train the model and collect basic performance metrics. We also introduce using TensorBoard to monitor training.

Chapter 12 explores and implements standard performance metrics and uses those metrics to identify weaknesses in the training done previously. We then mitigate those flaws with an improved training set that uses data balancing and augmentation.

Chapter 13 describes segmentation, a pixel-to-pixel model architecture that we use to produce a heatmap of possible nodule locations that covers the entire CT scan. This heatmap can be used to find nodules on CT scans for which we do not have human-annotated data.

Chapter 14 implements the final end-to-end project: diagnosis of cancer patients using our new segmentation model followed by classification.

PART 3

Part 3 is a single chapter on deployment. Chapter 15 provides an overview of how to deploy PyTorch models to a simple web service, embed them in a C++ program, or bring them to a mobile phone.

About the code

All of the code in this book was written for Python 3.6 or later. The code for the book is available for download from Manning's website (www.manning.com/books/deep-learning-with-pytorch) and on GitHub (https://github.com/deep-learning-with-pytorch/dlwpt-code). Version 3.6.8 was current at the time of writing and is what we used to test the examples in this book. For example:

```
$ python
Python 3.6.8 (default, Jan 14 2019, 11:02:34)
[GCC 8.0.1 20180414 on linux
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

Command lines intended to be entered at a Bash prompt start with `$` (for example, the `$ python` line in this example). Fixed-width inline code looks like `self`.

Code blocks that begin with >>> are transcripts of a session at the Python interactive prompt. The >>> characters are not meant to be considered input; text lines that

do not start with >>> or … are output. In some cases, an extra blank line is inserted before the >>> to improve readability in print. These blank lines are not included when you actually enter the text at the interactive prompt:

```
>>> print("Hello, world!")
Hello, world!

>>> print("Until next time...")
Until next time...
```

This blank line would not be present during an actual interactive session.

We also make heavy use of Jupyter Notebooks, as described in chapter 1, in section 1.5.1. Code from a notebook that we provide as part of the official GitHub repository looks like this:

```
# In[1]:
print("Hello, world!")

# Out[1]:
Hello, world!

# In[2]:
print("Until next time...")

# Out[2]:
Until next time...
```

Almost all of our example notebooks contain the following boilerplate in the first cell (some lines may be missing in early chapters), which we skip including in the book after this point:

```
# In[1]:
%matplotlib inline
from matplotlib import pyplot as plt
import numpy as np

import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim

torch.set_printoptions(edgeitems=2)
torch.manual_seed(123)
```

Otherwise, code blocks are partial or entire sections of .py source files.

Listing 15.1 main.py:5, `def main`

```
def main():
    print("Hello, world!")

if __name__ == '__main__':
    main()
```

Many of the code samples in the book are presented with two-space indents. Due to the limitations of print, code listings are limited to 80-character lines, which can be impractical for heavily indented sections of code. The use of two-space indents helps to mitigate the excessive line wrapping that would otherwise be present. All of the code available for download for the book (again, at www.manning.com/books/deep-learning-with-pytorch and https://github.com/deep-learning-with-pytorch/dlwpt-code) uses a consistent four-space indent. Variables named with a `_t` suffix are tensors stored in CPU memory, `_g` are tensors in GPU memory, and `_a` are NumPy arrays.

Hardware and software requirements

Part 1 has been designed to not require any particular computing resources. Any recent computer or online computing resource will be adequate. Similarly, no certain operating system is required. In part 2, we anticipate that completing a full training run for the more advanced examples will require a CUDA-capable GPU. The default parameters used in part 2 assume a GPU with 8 GB of RAM (we suggest an NVIDIA GTX 1070 or better), but the parameters can be adjusted if your hardware has less RAM available. The raw data needed for part 2's cancer-detection project is about 60 GB to download, and you will need a total of 200 GB (at minimum) of free disk space on the system that will be used for training. Luckily, online computing services recently started offering GPU time for free. We discuss computing requirements in more detail in the appropriate sections.

You need Python 3.6 or later; instructions can be found on the Python website (www.python.org/downloads). For PyTorch installation information, see the Get Started guide on the official PyTorch website (https://pytorch.org/get-started/locally). We suggest that Windows users install with Anaconda or Miniconda (https://www.anaconda.com/distribution or https://docs.conda.io/en/latest/miniconda.html). Other operating systems like Linux typically have a wider variety of workable options, with Pip being the most common package manager for Python. We provide a requirements.txt file that Pip can use to install dependencies. Since current Apple laptops do not include GPUs that support CUDA, the precompiled macOS packages for PyTorch are CPU-only. Of course, experienced users are free to install packages in the way that is most compatible with your preferred development environment.

liveBook discussion forum

Purchase of *Deep Learning with PyTorch* includes free access to a private web forum run by Manning Publications where you can make comments about the book, ask technical questions, and receive help from the authors and from other users. To access the forum, go to https://livebook.manning.com/#!/book/deep-learning-with-pytorch/discussion. You can learn more about Manning's forums and the rules of conduct at https://livebook.manning .com/#!/discussion. Manning's commitment to our readers is to provide a venue where a meaningful dialogue between individual readers and between readers and the author can take place. It is not a commitment to any specific

amount of participation on the part of the authors, whose contribution to the forum remains voluntary (and unpaid). We suggest you try asking them some challenging questions lest their interest stray! The forum and the archives of previous discussions will be accessible from the publisher's website as long as the book is in print.

Other online resources

Although this book does not assume prior knowledge of deep learning, it is not a foundational introduction to deep learning. We cover the basics, but our focus is on proficiency with the PyTorch library. We encourage interested readers to build up an intuitive understanding of deep learning either before, during, or after reading this book. Toward that end, *Grokking Deep Learning* (www.manning.com/books/grokking-deep-learning) is a great resource for developing a strong mental model and intuition about the mechanism underlying deep neural networks. For a thorough introduction and reference, we direct you to *Deep Learning* by Goodfellow et al. (www.deeplearningbook.org). And of course, Manning Publications has an extensive catalog of deep learning titles (www.manning.com/catalog#section-83) that cover a wide variety of topics in the space. Depending on your interests, many of them will make an excellent next book to read.

about the authors

Eli Stevens has spent the majority of his career working at startups in Silicon Valley, with roles ranging from software engineer (making enterprise networking appliances) to CTO (developing software for radiation oncology). At publication, he is working on machine learning in the self-driving-car industry.

Luca Antiga worked as a researcher in biomedical engineering in the 2000s, and spent the last decade as a cofounder and CTO of an AI engineering company. He has contributed to several open source projects, including the PyTorch core. He recently cofounded a US-based startup focused on infrastructure for data-defined software.

Thomas Viehmann is a machine learning and PyTorch specialty trainer and consultant based in Munich, Germany, and a PyTorch core developer. With a PhD in mathematics, he is not scared by theory, but he is thoroughly practical when applying it to computing challenges.

about the cover illustration

The figure on the cover of *Deep Learning with PyTorch* is captioned "Kardinian." The illustration is taken from a collection of dress costumes from various countries by Jacques Grasset de Saint-Sauveur (1757-1810), titled *Costumes civils actuels de tous les peuples connus,* published in France in 1788. Each illustration is finely drawn and colored by hand. The rich variety of Grasset de Saint-Sauveur's collection reminds us vividly of how culturally apart the world's towns and regions were just 200 years ago. Isolated from each other, people spoke different dialects and languages. In the streets or in the countryside, it was easy to identify where they lived and what their trade or station in life was just by their dress.

The way we dress has changed since then and the diversity by region, so rich at the time, has faded away. It is now hard to tell apart the inhabitants of different continents, let alone different towns, regions, or countries. Perhaps we have traded cultural diversity for a more varied personal life—certainly for a more varied and fast-paced technological life.

At a time when it is hard to tell one computer book from another, Manning celebrates the inventiveness and initiative of the computer business with book covers based on the rich diversity of regional life of two centuries ago, brought back to life by Grasset de Saint-Sauveur's pictures.

Part 1

Core PyTorch

Welcome to the first part of this book. This is where we'll take our first steps with PyTorch, gaining the fundamental skills needed to understand its anatomy and work out the mechanics of a PyTorch project.

In chapter 1, we'll make our first contact with PyTorch, understand what it is and what problems it solves, and how it relates to other deep learning frameworks. Chapter 2 will take us on a tour, giving us a chance to play with models that have been pretrained on fun tasks. Chapter 3 gets a bit more serious and teaches the basic data structure used in PyTorch programs: the tensor. Chapter 4 will take us on another tour, this time across ways to represent data from different domains as PyTorch tensors. Chapter 5 unveils how a program can learn from examples and how PyTorch supports this process. Chapter 6 provides the fundamentals of what a neural network is and how to build a neural network with PyTorch. Chapter 7 tackles a simple image classification problem with a neural network architecture. Finally, chapter 8 shows how the same problem can be cracked in a much smarter way using a convolutional neural network.

By the end of part 1, we'll have what it takes to tackle a real-world problem with PyTorch in part 2.

1 Introducing deep learning and the PyTorch Library

This chapter covers

- How deep learning changes our approach to machine learning
- Understanding why PyTorch is a good fit for deep learning
- Examining a typical deep learning project
- The hardware you'll need to follow along with the examples

The poorly defined term *artificial intelligence* covers a set of disciplines that have been subjected to a tremendous amount of research, scrutiny, confusion, fantastical hype, and sci-fi fearmongering. Reality is, of course, far more sanguine. It would be disingenuous to assert that today's machines are learning to "think" in any human sense of the word. Rather, we've discovered a general class of algorithms

that are able to approximate complicated, nonlinear processes very, very effectively, which we can use to automate tasks that were previously limited to humans.

For example, at https://talktotransformer.com, a language model called GPT-2 can generate coherent paragraphs of text one word at a time. When we fed it this very paragraph, it produced the following:

> *Next we're going to feed in a list of phrases from a corpus of email addresses, and see if the program can parse the lists as sentences. Again, this is much more complicated and far more complex than the search at the beginning of this post, but hopefully helps you understand the basics of constructing sentence structures in various programming languages.*

That's remarkably coherent for a machine, even if there isn't a well-defined thesis behind the rambling.

Even more impressively, the ability to perform these formerly human-only tasks is acquired *through examples*, rather than encoded by a human as a set of handcrafted rules. In a way, we're learning that intelligence is a notion we often conflate with self-awareness, and self-awareness is definitely not required to successfully carry out these kinds of tasks. In the end, the question of computer intelligence might not even be important. Edsger W. Dijkstra found that the question of whether machines could think was "about as relevant as the question of whether Submarines Can Swim."[1]

That general class of algorithms we're talking about falls under the AI subcategory of *deep learning*, which deals with training mathematical entities named *deep neural networks* by presenting instructive examples. Deep learning uses large amounts of data to approximate complex functions whose inputs and outputs are far apart, like an input image and, as output, a line of text describing the input; or a written script as input and a natural-sounding voice reciting the script as output; or, even more simply, associating an image of a golden retriever with a flag that tells us "Yes, a golden retriever is present." This kind of capability allows us to create programs with functionality that was, until very recently, exclusively the domain of human beings.

1.1 The deep learning revolution

To appreciate the paradigm shift ushered in by this deep learning approach, let's take a step back for a bit of perspective. Until the last decade, the broader class of systems that fell under the label *machine learning* relied heavily on *feature engineering*. Features are transformations on input data that facilitate a downstream algorithm, like a classifier, to produce correct outcomes on new data. Feature engineering consists of coming up with the right transformations so that the downstream algorithm can solve a task. For instance, in order to tell ones from zeros in images of handwritten digits, we would come up with a set of filters to estimate the direction of edges over the image, and then train a classifier to predict the correct digit given a distribution of edge directions. Another useful feature could be the number of enclosed holes, as seen in a zero, an eight, and, particularly, loopy twos.

[1] Edsger W. Dijkstra, "The Threats to Computing Science," http://mng.bz/nPJ5.

Deep learning, on the other hand, deals with finding such representations automatically, from raw data, in order to successfully perform a task. In the ones versus zeros example, filters would be refined during training by iteratively looking at pairs of examples and target labels. This is not to say that feature engineering has no place with deep learning; we often need to inject some form of prior knowledge in a learning system. However, the ability of a neural network to ingest data and extract useful representations on the basis of examples is what makes deep learning so powerful. The focus of deep learning practitioners is not so much on handcrafting those representations, but on operating on a mathematical entity so that it discovers representations from the training data autonomously. Often, these automatically created features are better than those that are handcrafted! As with many disruptive technologies, this fact has led to a change in perspective.

On the left side of figure 1.1, we see a practitioner busy defining engineering features and feeding them to a learning algorithm; the results on the task will be as good as the features the practitioner engineers. On the right, with deep learning, the raw data is fed to an algorithm that extracts hierarchical features automatically, guided by the optimization of its own performance on the task; the results will be as good as the ability of the practitioner to drive the algorithm toward its goal.

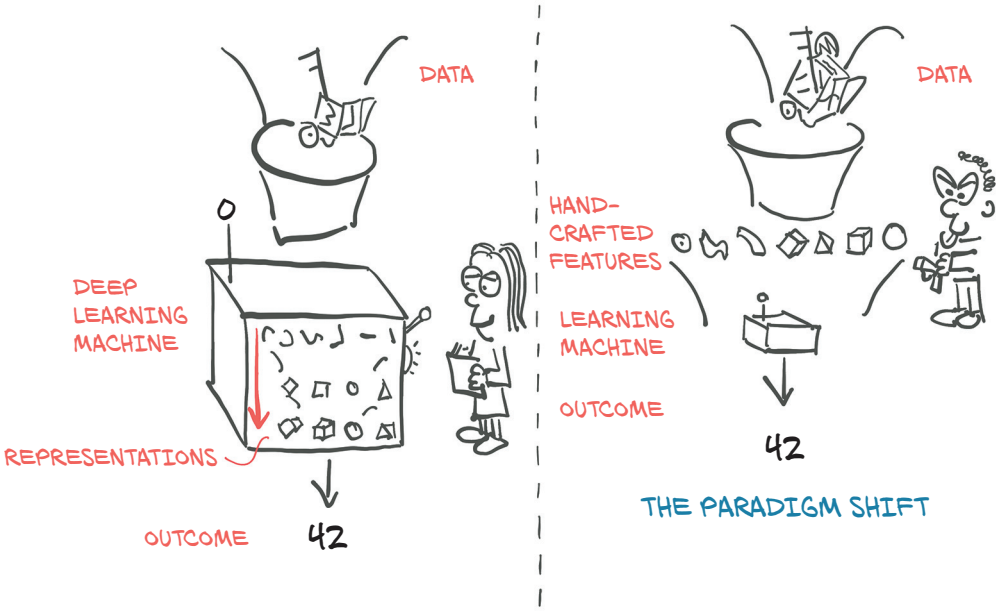


Figure 1.1 Deep learning exchanges the need to handcraft features for an increase in data and computational requirements.

Starting from the right side in figure 1.1, we already get a glimpse of what we need to execute successful deep learning:

- We need a way to ingest whatever data we have at hand.
- We somehow need to define the deep learning machine.
- We must have an automated way, *training*, to obtain useful representations and make the machine produce desired outputs.

This leaves us with taking a closer look at this training thing we keep talking about. During training, we use a *criterion*, a real-valued function of model outputs and reference data, to provide a numerical score for the discrepancy between the desired and actual output of our model (by convention, a lower score is typically better). Training consists of driving the criterion toward lower and lower scores by incrementally modifying our deep learning machine until it achieves low scores, even on data not seen during training.

1.2 PyTorch for deep learning

PyTorch is a library for Python programs that facilitates building deep learning projects. It emphasizes flexibility and allows deep learning models to be expressed in idiomatic Python. This approachability and ease of use found early adopters in the research community, and in the years since its first release, it has grown into one of the most prominent deep learning tools across a broad range of applications.

As Python does for programming, PyTorch provides an excellent introduction to deep learning. At the same time, PyTorch has been proven to be fully qualified for use in professional contexts for real-world, high-profile work. We believe that PyTorch's clear syntax, streamlined API, and easy debugging make it an excellent choice for introducing deep learning. We highly recommend studying PyTorch for your first deep learning library. Whether it ought to be the last deep learning library you learn is a decision we leave up to you.

At its core, the deep learning machine in figure 1.1 is a rather complex mathematical function mapping inputs to an output. To facilitate expressing this function, PyTorch provides a core data structure, the *tensor*, which is a multidimensional array that shares many similarities with NumPy arrays. Around that foundation, PyTorch comes with features to perform accelerated mathematical operations on dedicated hardware, which makes it convenient to design neural network architectures and train them on individual machines or parallel computing resources.

This book is intended as a starting point for software engineers, data scientists, and motivated students fluent in Python to become comfortable using PyTorch to build deep learning projects. We want this book to be as accessible and useful as possible, and we expect that you will be able to take the concepts in this book and apply them to other domains. To that end, we use a hands-on approach and encourage you to keep your computer at the ready, so you can play with the examples and take them a step further. By the time we are through with the book, we expect you to be able to

take a data source and build out a deep learning project with it, supported by the excellent official documentation.

Although we stress the practical aspects of building deep learning systems with PyTorch, we believe that providing an accessible introduction to a foundational deep learning tool is more than just a way to facilitate the acquisition of new technical skills. It is a step toward equipping a new generation of scientists, engineers, and practitioners from a wide range of disciplines with working knowledge that will be the backbone of many software projects during the decades to come.

In order to get the most out of this book, you will need two things:

- Some experience programming in Python. We're not going to pull any punches on that one; you'll need to be up on Python data types, classes, floating-point numbers, and the like.
- A willingness to dive in and get your hands dirty. We'll be starting from the basics and building up our working knowledge, and it will be much easier for you to learn if you follow along with us.

Deep Learning with PyTorch is organized in three distinct parts. Part 1 covers the foundations, examining in detail the facilities PyTorch offers to put the sketch of deep learning in figure 1.1 into action with code. Part 2 walks you through an end-to-end project involving medical imaging: finding and classifying tumors in CT scans, building on the basic concepts introduced in part 1, and adding more advanced topics. The short part 3 rounds off the book with a tour of what PyTorch offers for deploying deep learning models to production.

Deep learning is a huge space. In this book, we will be covering a tiny part of that space: specifically, using PyTorch for smaller-scope classification and segmentation projects, with image processing of 2D and 3D datasets used for most of the motivating examples. This book focuses on practical PyTorch, with the aim of covering enough ground to allow you to solve real-world machine learning problems, such as in vision, with deep learning or explore new models as they pop up in research literature. Most, if not all, of the latest publications related to deep learning research can be found in the arXiV public preprint repository, hosted at https://arxiv.org.[2]

1.3 Why PyTorch?

As we've said, deep learning allows us to carry out a very wide range of complicated tasks, like machine translation, playing strategy games, or identifying objects in cluttered scenes, by exposing our model to illustrative examples. In order to do so in practice, we need tools that are flexible, so they can be adapted to such a wide range of problems, and efficient, to allow training to occur over large amounts of data in reasonable times; and we need the trained model to perform correctly in the presence of variability in the inputs. Let's take a look at some of the reasons we decided to use PyTorch.

[2] We also recommend www.arxiv-sanity.com to help organize research papers of interest.

PyTorch is easy to recommend because of its simplicity. Many researchers and practitioners find it easy to learn, use, extend, and debug. It's Pythonic, and while like any complicated domain it has caveats and best practices, using the library generally feels familiar to developers who have used Python previously.

More concretely, programming the deep learning machine is very natural in PyTorch. PyTorch gives us a data type, the `Tensor`, to hold numbers, vectors, matrices, or arrays in general. In addition, it provides functions for operating on them. We can program with them incrementally and, if we want, interactively, just like we are used to from Python. If you know NumPy, this will be very familiar.

But PyTorch offers two things that make it particularly relevant for deep learning: first, it provides accelerated computation using graphical processing units (GPUs), often yielding speedups in the range of 50x over doing the same calculation on a CPU. Second, PyTorch provides facilities that support numerical optimization on generic mathematical expressions, which deep learning uses for training. Note that both features are useful for scientific computing in general, not exclusively for deep learning. In fact, we can safely characterize PyTorch as a high-performance library with optimization support for scientific computing in Python.

A design driver for PyTorch is expressivity, allowing a developer to implement complicated models without undue complexity being imposed by the library (it's not a framework!). PyTorch arguably offers one of the most seamless translations of ideas into Python code in the deep learning landscape. For this reason, PyTorch has seen widespread adoption in research, as witnessed by the high citation counts at international conferences.[3]

PyTorch also has a compelling story for the transition from research and development into production. While it was initially focused on research workflows, PyTorch has been equipped with a high-performance C++ runtime that can be used to deploy models for inference without relying on Python, and can be used for designing and training models in C++. It has also grown bindings to other languages and an interface for deploying to mobile devices. These features allow us to take advantage of PyTorch's flexibility and at the same time take our applications where a full Python runtime would be hard to get or would impose expensive overhead.

Of course, claims of ease of use and high performance are trivial to make. We hope that by the time you are in the thick of this book, you'll agree with us that our claims here are well founded.

1.3.1 The deep learning competitive landscape

While all analogies are flawed, it seems that the release of PyTorch 0.1 in January 2017 marked the transition from a Cambrian-explosion-like proliferation of deep learning libraries, wrappers, and data-exchange formats into an era of consolidation and unification.

[3] At the International Conference on Learning Representations (ICLR) 2019, PyTorch appeared as a citation in 252 papers, up from 87 the previous year and at the same level as TensorFlow, which appeared in 266 papers.

NOTE The deep learning landscape has been moving so quickly lately that by the time you read this in print, it will likely be out of date. If you're unfamiliar with some of the libraries mentioned here, that's fine.

At the time of PyTorch's first beta release:

- Theano and TensorFlow were the premiere low-level libraries, working with a model that had the user define a computational graph and then execute it.
- Lasagne and Keras were high-level wrappers around Theano, with Keras wrapping TensorFlow and CNTK as well.
- Caffe, Chainer, DyNet, Torch (the Lua-based precursor to PyTorch), MXNet, CNTK, DL4J, and others filled various niches in the ecosystem.

In the roughly two years that followed, the landscape changed drastically. The community largely consolidated behind either PyTorch or TensorFlow, with the adoption of other libraries dwindling, except for those filling specific niches. In a nutshell:

- Theano, one of the first deep learning frameworks, has ceased active development.
- TensorFlow:
  - Consumed Keras entirely, promoting it to a first-class API
  - Provided an immediate-execution "eager mode" that is somewhat similar to how PyTorch approaches computation
  - Released TF 2.0 with eager mode by default
- JAX, a library by Google that was developed independently from TensorFlow, has started gaining traction as a NumPy equivalent with GPU, autograd and JIT capabilities.
- PyTorch:
  - Consumed Caffe2 for its backend
  - Replaced most of the low-level code reused from the Lua-based Torch project
  - Added support for ONNX, a vendor-neutral model description and exchange format
  - Added a delayed-execution "graph mode" runtime called *TorchScript*
  - Released version 1.0
  - Replaced CNTK and Chainer as the framework of choice by their respective corporate sponsors

TensorFlow has a robust pipeline to production, an extensive industry-wide community, and massive mindshare. PyTorch has made huge inroads with the research and teaching communities, thanks to its ease of use, and has picked up momentum since, as researchers and graduates train students and move to industry. It has also built up steam in terms of production solutions. Interestingly, with the advent of TorchScript and eager mode, both PyTorch and TensorFlow have seen their feature sets start to converge with the other's, though the presentation of these features and the overall experience is still quite different between the two.

1.4 An overview of how PyTorch supports deep learning projects

We have already hinted at a few building blocks in PyTorch. Let's now take some time to formalize a high-level map of the main components that form PyTorch. We can best do this by looking at what a deep learning project needs from PyTorch.

First, PyTorch has the "Py" as in Python, but there's a lot of non-Python code in it. Actually, for performance reasons, most of PyTorch is written in C++ and CUDA (www.geforce.com/hardware/technology/cuda), a C++-like language from NVIDIA that can be compiled to run with massive parallelism on GPUs. There are ways to run PyTorch directly from C++, and we'll look into those in chapter 15. One of the motivations for this capability is to provide a reliable strategy for deploying models in production. However, most of the time we'll interact with PyTorch from Python, building models, training them, and using the trained models to solve actual problems.

Indeed, the Python API is where PyTorch shines in term of usability and integration with the wider Python ecosystem. Let's take a peek at the mental model of what PyTorch is.

As we already touched on, at its core, PyTorch is a library that provides *multidimensional arrays*, or *tensors* in PyTorch parlance (we'll go into details on those in chapter 3), and an extensive library of operations on them, provided by the `torch` module. Both tensors and the operations on them can be used on the CPU or the GPU. Moving computations from the CPU to the GPU in PyTorch doesn't require more than an additional function call or two. The second core thing that PyTorch provides is the ability of tensors to keep track of the operations performed on them and to analytically compute derivatives of an output of a computation with respect to any of its inputs. This is used for numerical optimization, and it is provided natively by tensors by virtue of dispatching through PyTorch's *autograd* engine under the hood.

By having tensors and the autograd-enabled tensor standard library, PyTorch can be used for physics, rendering, optimization, simulation, modeling, and more—we're very likely to see PyTorch used in creative ways throughout the spectrum of scientific applications. But PyTorch is first and foremost a deep learning library, and as such it provides all the building blocks needed to build neural networks and train them. Figure 1.2 shows a standard setup that loads data, trains a model, and then deploys that model to production.

The core PyTorch modules for building neural networks are located in `torch.nn`, which provides common neural network layers and other architectural components. Fully connected layers, convolutional layers, activation functions, and loss functions can all be found here (we'll go into more detail about what all that means as we go through the rest of this book). These components can be used to build and initialize the untrained model we see in the center of figure 1.2. In order to train our model, we need a few additional things: a source of training data, an optimizer to adapt the model to the training data, and a way to get the model and data to the hardware that will actually be performing the calculations needed for training the model.

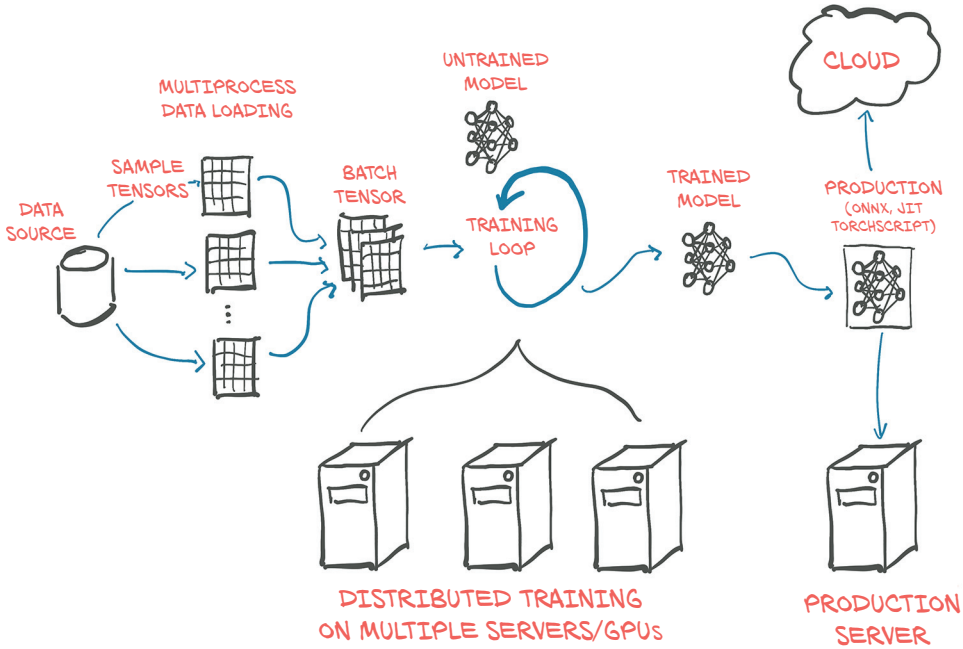


Figure 1.2 Basic, high-level structure of a PyTorch project, with data loading, training, and deployment to production

At left in figure 1.2, we see that quite a bit of data processing is needed before the training data even reaches our model.[4] First we need to physically get the data, most often from some sort of storage as the data source. Then we need to convert each sample from our data into a something PyTorch can actually handle: tensors. This bridge between our custom data (in whatever format it might be) and a standardized PyTorch tensor is the `Dataset` class PyTorch provides in `torch.utils.data`. As this process is wildly different from one problem to the next, we will have to implement this data sourcing ourselves. We will look in detail at how to represent various type of data we might want to work with as tensors in chapter 4.

As data storage is often slow, in particular due to access latency, we want to parallelize data loading. But as the many things Python is well loved for do not include easy, efficient, parallel processing, we will need multiple processes to load our data, in order to assemble them into *batches*: tensors that encompass several samples. This is rather elaborate; but as it is also relatively generic, PyTorch readily provides all that magic in the `DataLoader` class. Its instances can spawn child processes to load data from a dataset in the background so that it's ready and waiting for the training loop as soon as the loop can use it. We will meet and use `Dataset` and `DataLoader` in chapter 7.

[4] And that's just the data preparation that is done on the fly, not the preprocessing, which can be a pretty large part in practical projects.

With the mechanism for getting batches of samples in place, we can turn to the training loop itself at the center of figure 1.2. Typically, the training loop is implemented as a standard Python `for` loop. In the simplest case, the model runs the required calculations on the local CPU or a single GPU, and once the training loop has the data, computation can start immediately. Chances are this will be your basic setup, too, and it's the one we'll assume in this book.

At each step in the training loop, we evaluate our model on the samples we got from the data loader. We then compare the outputs of our model to the desired output (the targets) using some *criterion* or *loss function*. Just as it offers the components from which to build our model, PyTorch also has a variety of loss functions at our disposal. They, too, are provided in `torch.nn`. After we have compared our actual outputs to the ideal with the loss functions, we need to push the model a little to move its outputs to better resemble the target. As mentioned earlier, this is where the PyTorch autograd engine comes in; but we also need an *optimizer* doing the updates, and that is what PyTorch offers us in `torch.optim`. We will start looking at training loops with loss functions and optimizers in chapter 5 and then hone our skills in chapters 6 through 8 before embarking on our big project in part 2.

It's increasingly common to use more elaborate hardware like multiple GPUs or multiple machines that contribute their resources to training a large model, as seen in the bottom center of figure 1.2. In those cases, `torch.nn.parallel.DistributedDataParallel` and the `torch.distributed` submodule can be employed to use the additional hardware.

The training loop might be the most unexciting yet most time-consuming part of a deep learning project. At the end of it, we are rewarded with a model whose parameters have been optimized on our task: the *trained model* depicted to the right of the training loop in the figure. Having a model to solve a task is great, but in order for it to be useful, we must put it where the work is needed. This *deployment* part of the process, depicted on the right in figure 1.2, may involve putting the model on a server or exporting it to load it to a cloud engine, as shown in the figure. Or we might integrate it with a larger application, or run it on a phone.

One particular step of the deployment exercise can be to export the model. As mentioned earlier, PyTorch defaults to an immediate execution model (eager mode). Whenever an instruction involving PyTorch is executed by the Python interpreter, the corresponding operation is immediately carried out by the underlying C++ or CUDA implementation. As more instructions operate on tensors, more operations are executed by the backend implementation.

PyTorch also provides a way to compile models ahead of time through *TorchScript*. Using TorchScript, PyTorch can serialize a model into a set of instructions that can be invoked independently from Python: say, from C++ programs or on mobile devices. We can think about it as a virtual machine with a limited instruction set, specific to tensor operations. This allows us to export our model, either as TorchScript to be used with the PyTorch runtime, or in a standardized format called *ONNX*. These features are at

the basis of the production deployment capabilities of PyTorch. We'll cover this in chapter 15.

1.5 Hardware and software requirements

This book will require coding and running tasks that involve heavy numerical computing, such as multiplication of large numbers of matrices. As it turns out, running a pretrained network on new data is within the capabilities of any recent laptop or personal computer. Even taking a pretrained network and retraining a small portion of it to specialize it on a new dataset doesn't necessarily require specialized hardware. You can follow along with everything we do in part 1 of this book using a standard personal computer or laptop.

However, we anticipate that completing a full training run for the more advanced examples in part 2 will require a CUDA-capable GPU. The default parameters used in part 2 assume a GPU with 8 GB of RAM (we suggest an NVIDIA GTX 1070 or better), but those can be adjusted if your hardware has less RAM available. To be clear: such hardware is not mandatory if you're willing to wait, but running on a GPU cuts training time by at least an order of magnitude (and usually it's 40–50x faster). Taken individually, the operations required to compute parameter updates are fast (from fractions of a second to a few seconds) on modern hardware like a typical laptop CPU. The issue is that training involves running these operations over and over, many, many times, incrementally updating the network parameters to minimize the training error.

Moderately large networks can take hours to days to train from scratch on large, real-world datasets on workstations equipped with a good GPU. That time can be reduced by using multiple GPUs on the same machine, and even further on clusters of machines equipped with multiple GPUs. These setups are less prohibitive to access than it sounds, thanks to the offerings of cloud computing providers. DAWNBench (https://dawn.cs.stanford.edu/benchmark/index.html) is an interesting initiative from Stanford University aimed at providing benchmarks on training time and cloud computing costs related to common deep learning tasks on publicly available datasets.

So, if there's a GPU around by the time you reach part 2, then great. Otherwise, we suggest checking out the offerings from the various cloud platforms, many of which offer GPU-enabled Jupyter Notebooks with PyTorch preinstalled, often with a free quota. Google Colaboratory (https://colab.research.google.com) is a great place to start.

The last consideration is the operating system (OS). PyTorch has supported Linux and macOS from its first release, and it gained Windows support in 2018. Since current Apple laptops do not include GPUs that support CUDA, the precompiled macOS packages for PyTorch are CPU-only. Throughout the book, we will try to avoid assuming you are running a particular OS, although some of the scripts in part 2 are shown as if running from a Bash prompt under Linux. Those scripts' command lines should convert to a Windows-compatible form readily. For convenience, code will be listed as if running from a Jupyter Notebook when possible.

For installation information, please see the Get Started guide on the official PyTorch website (https://pytorch.org/get-started/locally). We suggest that Windows users install with Anaconda or Miniconda (https://www.anaconda.com/distribution or https://docs.conda.io/en/latest/miniconda.html). Other operating systems like Linux typically have a wider variety of workable options, with Pip being the most common package manager for Python. We provide a requirements.txt file that pip can use to install dependencies. Of course, experienced users are free to install packages in the way that is most compatible with your preferred development environment.

Part 2 has some nontrivial download bandwidth and disk space requirements as well. The raw data needed for the cancer-detection project in part 2 is about 60 GB to download, and when uncompressed it requires about 120 GB of space. The compressed data can be removed after decompressing it. In addition, due to caching some of the data for performance reasons, another 80 GB will be needed while training. You will need a total of 200 GB (at minimum) of free disk space on the system that will be used for training. While it is possible to use network storage for this, there might be training speed penalties if the network access is slower than local disk. Preferably you will have space on a local SSD to store the data for fast retrieval.

1.5.1 Using Jupyter Notebooks

We're going to assume you've installed PyTorch and the other dependencies and have verified that things are working. Earlier we touched on the possibilities for following along with the code in the book. We are going to be making heavy use of Jupyter Notebooks for our example code. A Jupyter Notebook shows itself as a page in the browser through which we can run code interactively. The code is evaluated by a *kernel*, a process running on a server that is ready to receive code to execute and send back the results, which are then rendered inline on the page. A notebook maintains the state of the kernel, like variables defined during the evaluation of code, in memory until it is terminated or restarted. The fundamental unit with which we interact with a notebook is a *cell*: a box on the page where we can type code and have the kernel evaluate it (through the menu item or by pressing Shift-Enter). We can add multiple cells in a notebook, and the new cells will see the variables we created in the earlier cells. The value returned by the last line of a cell will be printed right below the cell after execution, and the same goes for plots. By mixing source code, results of evaluations, and Markdown-formatted text cells, we can generate beautiful interactive documents. You can read everything about Jupyter Notebooks on the project website (https://jupyter.org).

At this point, you need to start the notebook server from the root directory of the code checkout from GitHub. How exactly starting the server looks depends on the details of your OS and how and where you installed Jupyter. If you have questions, feel free to ask on the book's forum.[5] Once started, your default browser will pop up, showing a list of local notebook files.

[5] https://forums.manning.com/forums/deep-learning-with-pytorch

NOTE Jupyter Notebooks are a powerful tool for expressing and investigating ideas through code. While we think that they make for a good fit for our use case with this book, they're not for everyone. We would argue that it's important to focus on removing friction and minimizing cognitive overhead, and that's going to be different for everyone. Use what you like during your experimentation with PyTorch.

Full working code for all listings from the book can be found at the book's website (www.manning.com/books/deep-learning-with-pytorch) and in our repository on GitHub (https://github.com/deep-learning-with-pytorch/dlwpt-code).

1.6 Exercises

1. Start Python to get an interactive prompt.
   a. What Python version are you using? We hope it is at least 3.6!
   b. Can you `import torch`? What version of PyTorch do you get?
   c. What is the result of `torch.cuda.is_available()`? Does it match your expectation based on the hardware you're using?
2. Start the Jupyter notebook server.
   a. What version of Python is Jupyter using?
   b. Is the location of the `torch` library used by Jupyter the same as the one you imported from the interactive prompt?

1.7 Summary

- Deep learning models automatically learn to associate inputs and desired outputs from examples.
- Libraries like PyTorch allow you to build and train neural network models efficiently.
- PyTorch minimizes cognitive overhead while focusing on flexibility and speed. It also defaults to immediate execution for operations.
- TorchScript allows us to precompile models and invoke them not only from Python but also from C++ programs and on mobile devices.
- Since the release of PyTorch in early 2017, the deep learning tooling ecosystem has consolidated significantly.
- PyTorch provides a number of utility libraries to facilitate deep learning projects.

2 Pretrained networks

This chapter covers

- Running pretrained image-recognition models
- An introduction to GANs and CycleGAN
- Captioning models that can produce text descriptions of images
- Sharing models through Torch Hub

We closed our first chapter promising to unveil amazing things in this chapter, and now it's time to deliver. Computer vision is certainly one of the fields that have been most impacted by the advent of deep learning, for a variety of reasons. The need to classify or interpret the content of natural images existed, very large datasets became available, and new constructs such as convolutional layers were invented and could be run quickly on GPUs with unprecedented accuracy. All of these factors combined with the internet giants' desire to understand pictures taken by millions of users with their mobile devices and managed on said giants' platforms. Quite the perfect storm.

We are going to learn how to use the work of the best researchers in the field by downloading and running very interesting models that have already been trained on open, large-scale datasets. We can think of a pretrained neural network as similar to

a program that takes inputs and generates outputs. The behavior of such a program is dictated by the architecture of the neural network and by the examples it saw during training, in terms of desired input-output pairs, or desired properties that the output should satisfy. Using an off-the-shelf model can be a quick way to jump-start a deep learning project, since it draws on expertise from the researchers who designed the model, as well as the computation time that went into training the weights.

In this chapter, we will explore three popular pretrained models: a model that can label an image according to its content, another that can fabricate a new image from a real image, and a model that can describe the content of an image using proper English sentences. We will learn how to load and run these pretrained models in PyTorch, and we will introduce PyTorch Hub, a set of tools through which PyTorch models like the pretrained ones we'll discuss can be easily made available through a uniform interface. Along the way, we'll discuss data sources, define terminology like *label*, and attend a zebra rodeo.

If you're coming to PyTorch from another deep learning framework, and you'd rather jump right into learning the nuts and bolts of PyTorch, you can get away with skipping to the next chapter. The things we'll cover in this chapter are more fun than foundational and are somewhat independent of any given deep learning tool. That's not to say they're not important! But if you've worked with pretrained models in other deep learning frameworks, then you already know how powerful a tool they can be. And if you're already familiar with the generative adversarial network (GAN) game, you don't need us to explain it to you.

We hope you keep reading, though, since this chapter hides some important skills under the fun. Learning how to run a pretrained model using PyTorch is a useful skill—full stop. It's especially useful if the model has been trained on a large dataset. We will need to get accustomed to the mechanics of obtaining and running a neural network on real-world data, and then visualizing and evaluating its outputs, whether we trained it or not.

2.1 A pretrained network that recognizes the subject of an image

As our first foray into deep learning, we'll run a state-of-the-art deep neural network that was pretrained on an object-recognition task. There are many pretrained networks that can be accessed through source code repositories. It is common for researchers to publish their source code along with their papers, and often the code comes with weights that were obtained by training a model on a reference dataset. Using one of these models could enable us to, for example, equip our next web service with image-recognition capabilities with very little effort.

The pretrained network we'll explore here was trained on a subset of the ImageNet dataset (http://imagenet.stanford.edu). ImageNet is a very large dataset of over 14 million images maintained by Stanford University. All of the images are labeled with a hierarchy of nouns that come from the WordNet dataset (http://wordnet.princeton.edu), which is in turn a large lexical database of the English language.

The ImageNet dataset, like several other public datasets, has its origin in academic competitions. Competitions have traditionally been some of the main playing fields where researchers at institutions and companies regularly challenge each other. Among others, the ImageNet Large Scale Visual Recognition Challenge (ILSVRC) has gained popularity since its inception in 2010. This particular competition is based on a few tasks, which can vary each year, such as image classification (telling what object categories the image contains), object localization (identifying objects' position in images), object detection (identifying and labeling objects in images), scene classification (classifying a situation in an image), and scene parsing (segmenting an image into regions associated with semantic categories, such as cow, house, cheese, hat). In particular, the image-classification task consists of taking an input image and producing a list of 5 labels out of 1,000 total categories, ranked by confidence, describing the content of the image.

The training set for ILSVRC consists of 1.2 million images labeled with one of 1,000 nouns (for example, "dog"), referred to as the *class* of the image. In this sense, we will use the terms *label* and *class* interchangeably. We can take a peek at images from ImageNet in figure 2.1.

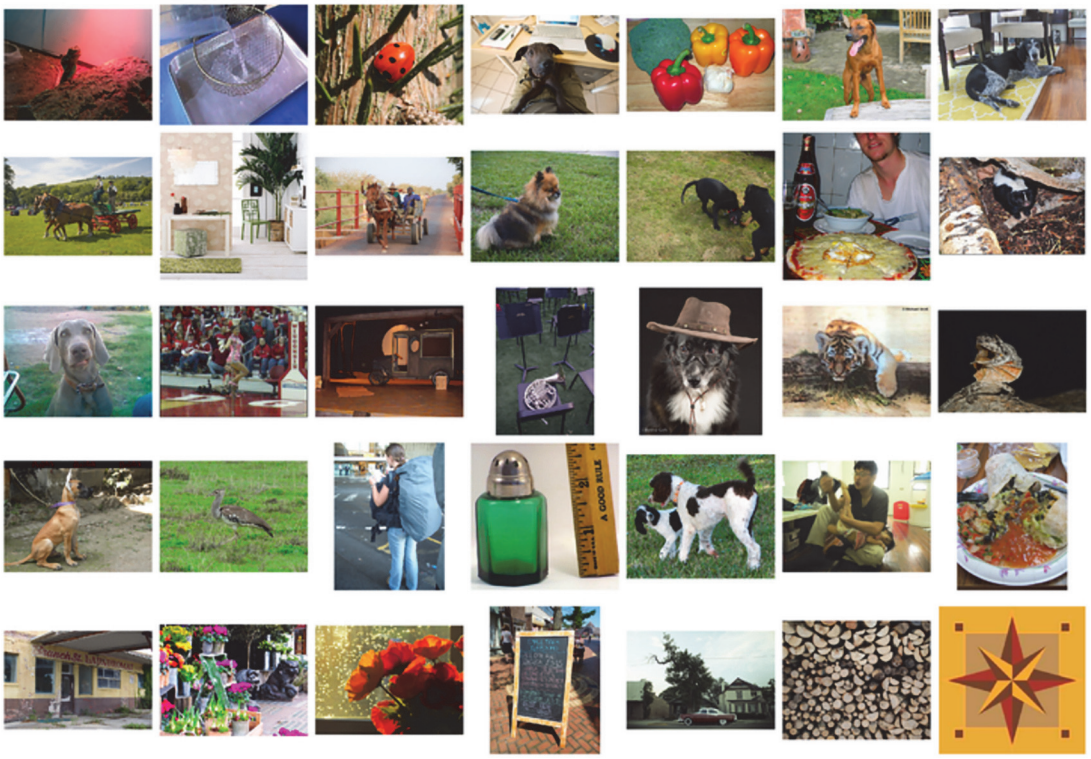


Figure 2.1 A small sample of ImageNet images

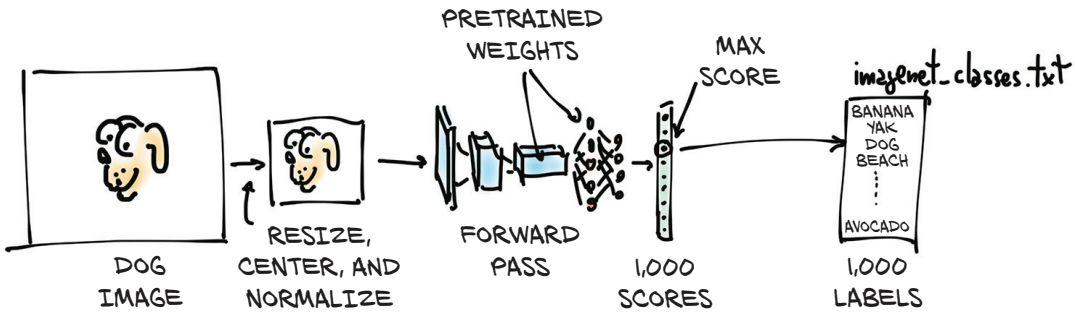


Figure 2.2 The inference process

We are going to end up being able to take our own images and feed them into our pretrained model, as pictured in figure 2.2. This will result in a list of predicted labels for that image, which we can then examine to see what the model thinks our image is. Some images will have predictions that are accurate, and others will not!

The input image will first be preprocessed into an instance of the multidimensional array class `torch.Tensor`. It is an RGB image with height and width, so this tensor will have three dimensions: the three color channels, and two spatial image dimensions of a specific size. (We'll get into the details of what a tensor is in chapter 3, but for now, think of it as being like a vector or matrix of floating-point numbers.) Our model will take that processed input image and pass it into the pretrained network to obtain scores for each class. The highest score corresponds to the most likely class according to the weights. Each class is then mapped one-to-one onto a class label. That output is contained in a `torch.Tensor` with 1,000 elements, each representing the score associated with that class.

Before we can do all that, we'll need to get the network itself, take a peek under the hood to see how it's structured, and learn about how to prepare our data before the model can use it.

2.1.1 Obtaining a pretrained network for image recognition

As discussed, we will now equip ourselves with a network trained on ImageNet. To do so, we'll take a look at the TorchVision project (https://github.com/pytorch/vision), which contains a few of the best-performing neural network architectures for computer vision, such as AlexNet (http://mng.bz/lo6z), ResNet (https://arxiv.org/pdf/1512.03385.pdf), and Inception v3 (https://arxiv.org/pdf/1512.00567.pdf). It also has easy access to datasets like ImageNet and other utilities for getting up to speed with computer vision applications in PyTorch. We'll dive into some of these further along in the book. For now, let's load up and run two networks: first AlexNet, one of the early breakthrough networks for image recognition; and then a residual network, ResNet for short, which won the ImageNet classification, detection, and localization

competitions, among others, in 2015. If you didn't get PyTorch up and running in chapter 1, now is a good time to do that.

The predefined models can be found in `torchvision.models` (code/p1ch2/2_pre_trained_networks.ipynb):

```
# In[1]:
from torchvision import models
```

We can take a look at the actual models:

```
# In[2]:
dir(models)

# Out[2]:
['AlexNet',
 'DenseNet',
 'Inception3',
 'ResNet',
 'SqueezeNet',
 'VGG',
...
 'alexnet',
 'densenet',
 'densenet121',
...
 'resnet',
 'resnet101',
 'resnet152',
...
 ]
```

The capitalized names refer to Python classes that implement a number of popular models. They differ in their architecture—that is, in the arrangement of the operations occurring between the input and the output. The lowercase names are convenience functions that return models instantiated from those classes, sometimes with different parameter sets. For instance, `resnet101` returns an instance of `ResNet` with 101 layers, `resnet18` has 18 layers, and so on. We'll now turn our attention to AlexNet.

2.1.2 AlexNet

The AlexNet architecture won the 2012 ILSVRC by a large margin, with a top-5 test error rate (that is, the correct label must be in the top 5 predictions) of 15.4%. By comparison, the second-best submission, which wasn't based on a deep network, trailed at 26.2%. This was a defining moment in the history of computer vision: the moment when the community started to realize the potential of deep learning for vision tasks. That leap was followed by constant improvement, with more modern architectures and training methods getting top-5 error rates as low as 3%.

By today's standards, AlexNet is a rather small network, compared to state-of-the-art models. But in our case, it's perfect for taking a first peek at a neural network that does something and learning how to run a pretrained version of it on a new image.

We can see the structure of AlexNet in figure 2.3. Not that we have all the elements for understanding it now, but we can anticipate a few aspects. First, each block consists of a bunch of multiplications and additions, plus a sprinkle of other functions in the output that we'll discover in chapter 5. We can think of it as a filter—a function that takes one or more images as input and produces other images as output. The way it does so is determined during training, based on the examples it has *seen* and on the desired outputs for those.

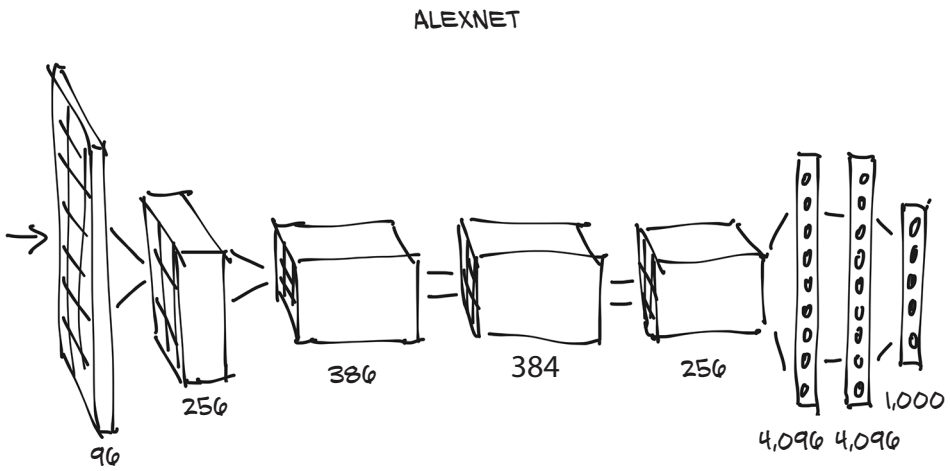


Figure 2.3 The AlexNet architecture

In figure 2.3, input images come in from the left and go through five stacks of filters, each producing a number of output images. After each filter, the images are reduced in size, as annotated. The images produced by the last stack of filters are laid out as a 4,096-element 1D vector and classified to produce 1,000 output probabilities, one for each output class.

In order to run the AlexNet architecture on an input image, we can create an instance of the `AlexNet` class. This is how it's done:

```
# In[3]:
alexnet = models.AlexNet()
```

At this point, `alexnet` is an object that can run the AlexNet architecture. It's not essential for us to understand the details of this architecture for now. For the time being, `AlexNet` is just an opaque object that can be called like a function. By providing

`alexnet` with some precisely sized input data (we'll see shortly what this input data should be), we will run a *forward pass* through the network. That is, the input will run through the first set of neurons, whose outputs will be fed to the next set of neurons, all the way to the final output. Practically speaking, assuming we have an `input` object of the right type, we can run the forward pass with `output = alexnet(input)`.

But if we did that, we would be feeding data through the whole network to produce … garbage! That's because the network is uninitialized: its weights, the numbers by which inputs are added and multiplied, have not been trained on anything—the network itself is a blank (or rather, *random*) slate. We'd need to either train it from scratch or load weights from prior training, which we'll do now.

To this end, let's go back to the `models` module. We learned that the uppercase names correspond to classes that implement popular architectures for computer vision. The lowercase names, on the other hand, are functions that instantiate models with predefined numbers of layers and units and optionally download and load pretrained weights into them. Note that there's nothing essential about using one of these functions: they just make it convenient to instantiate the model with a number of layers and units that matches how the pretrained networks were built.

2.1.3 ResNet

Using the `resnet101` function, we'll now instantiate a 101-layer convolutional neural network. Just to put things in perspective, before the advent of residual networks in 2015, achieving stable training at such depths was considered extremely hard. Residual networks pulled a trick that made it possible, and by doing so, beat several benchmarks in one sweep that year.

Let's create an instance of the network now. We'll pass an argument that will instruct the function to download the weights of `resnet101` trained on the ImageNet dataset, with 1.2 million images and 1,000 categories:

```
# In[4]:
resnet = models.resnet101(pretrained=True)
```

While we're staring at the download progress, we can take a minute to appreciate that `resnet101` sports 44.5 million parameters—that's a lot of parameters to optimize automatically!

2.1.4 Ready, set, almost run

OK, what did we just get? Since we're curious, we'll take a peek at what a `resnet101` looks like. We can do so by printing the value of the returned model. This gives us a textual representation of the same kind of information we saw in 2.3, providing details about the structure of the network. For now, this will be information overload, but as we progress through the book, we'll increase our ability to understand what this code is telling us:

```
# In[5]:
resnet

# Out[5]:
ResNet(
  (conv1): Conv2d(3, 64, kernel_size=(7, 7), stride=(2, 2), padding=(3, 3),
                  bias=False)
  (bn1): BatchNorm2d(64, eps=1e-05, momentum=0.1, affine=True,
                     track_running_stats=True)
  (relu): ReLU(inplace)
  (maxpool): MaxPool2d(kernel_size=3, stride=2, padding=1, dilation=1,
                       ceil_mode=False)
  (layer1): Sequential(
    (0): Bottleneck(
...
    )
  )
  (avgpool): AvgPool2d(kernel_size=7, stride=1, padding=0)
  (fc): Linear(in_features=2048, out_features=1000, bias=True)
)
```

What we are seeing here is `modules`, one per line. Note that they have nothing in common with Python modules: they are individual operations, the building blocks of a neural network. They are also called *layers* in other deep learning frameworks.

If we scroll down, we'll see a lot of `Bottleneck` modules repeating one after the other (101 of them!), containing convolutions and other modules. That's the anatomy of a typical deep neural network for computer vision: a more or less sequential cascade of filters and nonlinear functions, ending with a layer (`fc`) producing scores for each of the 1,000 output classes (`out_features`).

The `resnet` variable can be called like a function, taking as input one or more images and producing an equal number of scores for each of the 1,000 ImageNet classes. Before we can do that, however, we have to preprocess the input images so they are the right size and so that their values (colors) sit roughly in the same numerical range. In order to do that, the `torchvision` module provides `transforms`, which allow us to quickly define pipelines of basic preprocessing functions:

```
# In[6]:
from torchvision import transforms
preprocess = transforms.Compose([
        transforms.Resize(256),
        transforms.CenterCrop(224),
        transforms.ToTensor(),
        transforms.Normalize(
            mean=[0.485, 0.456, 0.406],
            std=[0.229, 0.224, 0.225]
        )])
```

In this case, we defined a `preprocess` function that will scale the input image to 256 × 256, crop the image to 224 × 224 around the center, transform it to a tensor (a PyTorch multidimensional array: in this case, a 3D array with color, height, and

width), and normalize its RGB (red, green, blue) components so that they have defined means and standard deviations. These need to match what was presented to the network during training, if we want the network to produce meaningful answers. We'll go into more depth about transforms when we dive into making our own image-recognition models in section 7.1.3.

We can now grab a picture of our favorite dog (say, bobby.jpg from the GitHub repo), preprocess it, and then see what ResNet thinks of it. We can start by loading an image from the local filesystem using Pillow (https://pillow.readthedocs.io/en/stable), an image-manipulation module for Python:

```
# In[7]:
from PIL import Image
img = Image.open("../data/p1ch2/bobby.jpg")
```

If we were following along from a Jupyter Notebook, we would do the following to see the picture inline (it would be shown where the `<PIL.JpegImagePlugin…` is in the following):

```
# In[8]:
img
# Out[8]:
<PIL.JpegImagePlugin.JpegImageFile image mode=RGB size=1280x720 at
 0x1B1601360B8>
```

Otherwise, we can invoke the `show` method, which will pop up a window with a viewer, to see the image shown in figure 2.4:

```
>>> img.show()
```

Figure 2.4 Bobby, our very special input image

Next, we can pass the image through our preprocessing pipeline:

```
# In[9]:
img_t = preprocess(img)
```

Then we can reshape, crop, and normalize the input tensor in a way that the network expects. We'll understand more of this in the next two chapters; hold tight for now:

```
# In[10]:
import torch
batch_t = torch.unsqueeze(img_t, 0)
```

We're now ready to run our model.

2.1.5 Run!

The process of running a trained model on new data is called *inference* in deep learning circles. In order to do inference, we need to put the network in `eval` mode:

```
# In[11]:
resnet.eval()

# Out[11]:
ResNet(
  (conv1): Conv2d(3, 64, kernel_size=(7, 7), stride=(2, 2), padding=(3, 3),
                  bias=False)
  (bn1): BatchNorm2d(64, eps=1e-05, momentum=0.1, affine=True,
                     track_running_stats=True)
  (relu): ReLU(inplace)
  (maxpool): MaxPool2d(kernel_size=3, stride=2, padding=1, dilation=1,
                       ceil_mode=False)
  (layer1): Sequential(
    (0): Bottleneck(
...
    )
  )
  (avgpool): AvgPool2d(kernel_size=7, stride=1, padding=0)
  (fc): Linear(in_features=2048, out_features=1000, bias=True)
)
```

If we forget to do that, some pretrained models, like *batch normalization* and *dropout*, will not produce meaningful answers, just because of the way they work internally. Now that `eval` has been set, we're ready for inference:

```
# In[12]:
out = resnet(batch_t)
out

# Out[12]:
tensor([[ -3.4803,  -1.6618,  -2.4515,  -3.2662,  -3.2466,  -1.3611,
          -2.0465,  -2.5112,  -1.3043,  -2.8900,  -1.6862,  -1.3055,
...
           2.8674,  -3.7442,   1.5085,  -3.2500,  -2.4894,  -0.3354,
           0.1286,  -1.1355,   3.3969,   4.4584]])
```

A staggering set of operations involving 44.5 million parameters has just happened, producing a vector of 1,000 scores, one per ImageNet class. That didn't take long, did it?

We now need to find out the label of the class that received the highest score. This will tell us what the model saw in the image. If the label matches how a human would describe the image, that's great! It means everything is working. If not, then either something went wrong during training, or the image is so different from what the model expects that the model can't process it properly, or there's some other similar issue.

To see the list of predicted labels, we will load a text file listing the labels in the same order they were presented to the network during training, and then we will pick out the label at the index that produced the highest score from the network. Almost all models meant for image recognition have output in a form similar to what we're about to work with.

Let's load the file containing the 1,000 labels for the ImageNet dataset classes:

```
# In[13]:
with open('../data/p1ch2/imagenet_classes.txt') as f:
    labels = [line.strip() for line in f.readlines()]
```

At this point, we need to determine the index corresponding to the maximum score in the `out` tensor we obtained previously. We can do that using the `max` function in PyTorch, which outputs the maximum value in a tensor as well as the indices where that maximum value occurred:

```
# In[14]:
_, index = torch.max(out, 1)
```

We can now use the index to access the label. Here, `index` is not a plain Python number, but a one-element, one-dimensional tensor (specifically, `tensor([207])`), so we need to get the actual numerical value to use as an index into our `labels` list using `index[0]`. We also use `torch.nn.functional.softmax` (http://mng.bz/BYnq) to normalize our outputs to the range [0, 1], and divide by the sum. That gives us something roughly akin to the confidence that the model has in its prediction. In this case, the model is 96% certain that it knows what it's looking at is a golden retriever:

```
# In[15]:
percentage = torch.nn.functional.softmax(out, dim=1)[0] * 100
labels[index[0]], percentage[index[0]].item()

# Out[15]:
('golden retriever', 96.29334259033203)
```

Uh oh, who's a good boy?

Since the model produced scores, we can also find out what the second best, third best, and so on were. To do this, we can use the `sort` function, which sorts the values in ascending or descending order and also provides the indices of the sorted values in the original array:

```
# In[16]:
_, indices = torch.sort(out, descending=True)
[(labels[idx], percentage[idx].item()) for idx in indices[0][:5]]

# Out[16]:
[('golden retriever', 96.29334259033203),
 ('Labrador retriever', 2.80812406539917),
 ('cocker spaniel, English cocker spaniel, cocker', 0.28267428278923035),
 ('redbone', 0.2086310237646103),
 ('tennis ball', 0.11621569097042084)]
```

We see that the first four are dogs (redbone is a breed; who knew?), after which things start to get funny. The fifth answer, "tennis ball," is probably because there are enough pictures of tennis balls with dogs nearby that the model is essentially saying, "There's a 0.1% chance that I've completely misunderstood what a tennis ball is." This is a great example of the fundamental differences in how humans and neural networks view the world, as well as how easy it is for strange, subtle biases to sneak into our data.

Time to play! We can go ahead and interrogate our network with random images and see what it comes up with. How successful the network will be will largely depend on whether the subjects were well represented in the training set. If we present an image containing a subject outside the training set, it's quite possible that the network will come up with a wrong answer with pretty high confidence. It's useful to experiment and get a feel for how a model reacts to unseen data.

We've just run a network that won an image-classification competition in 2015. It learned to recognize our dog from examples of dogs, together with a ton of other real-world subjects. We'll now see how different architectures can achieve other kinds of tasks, starting with image generation.

2.2 A pretrained model that fakes it until it makes it

Let's suppose, for a moment, that we're career criminals who want to move into selling forgeries of "lost" paintings by famous artists. We're criminals, not painters, so as we paint our fake Rembrandts and Picassos, it quickly becomes apparent that they're amateur imitations rather than the real deal. Even if we spend a bunch of time practicing until we get a canvas that *we* can't tell is fake, trying to pass it off at the local art auction house is going to get us kicked out instantly. Even worse, being told "This is clearly fake; get out," doesn't help us improve! We'd have to randomly try a bunch of things, gauge which ones took *slightly* longer to recognize as forgeries, and emphasize those traits on our future attempts, which would take far too long.

Instead, we need to find an art historian of questionable moral standing to inspect our work and tell us exactly what it was that tipped them off that the painting wasn't legit. With that feedback, we can improve our output in clear, directed ways, until our sketchy scholar can no longer tell our paintings from the real thing.

Soon, we'll have our "Botticelli" in the Louvre, and their Benjamins in our pockets. We'll be rich!

While this scenario is a bit farcical, the underlying technology is sound and will likely have a profound impact on the perceived veracity of digital data in the years to come. The entire concept of "photographic evidence" is likely to become entirely suspect, given how easy it will be to automate the production of convincing, yet fake, images and video. The only key ingredient is data. Let's see how this process works.

2.2.1 The GAN game

In the context of deep learning, what we've just described is known as *the GAN game*, where two networks, one acting as the painter and the other as the art historian, compete to outsmart each other at creating and detecting forgeries. GAN stands for *generative adversarial network*, where *generative* means something is being created (in this case, fake masterpieces), *adversarial* means the two networks are competing to outsmart the other, and well, *network* is pretty obvious. These networks are one of the most original outcomes of recent deep learning research.

Remember that our overarching goal is to produce synthetic examples of a class of images that cannot be recognized as fake. When mixed in with legitimate examples, a skilled examiner would have trouble determining which ones are real and which are our forgeries.

The *generator* network takes the role of the painter in our scenario, tasked with producing realistic-looking images, starting from an arbitrary input. The *discriminator* network is the amoral art inspector, needing to tell whether a given image was fabricated by the generator or belongs in a set of real images. This two-network design is atypical for most deep learning architectures but, when used to implement a GAN game, can lead to incredible results.

Figure 2.5 shows a rough picture of what's going on. The end goal for the generator is to fool the discriminator into mixing up real and fake images. The end goal for the discriminator is to find out when it's being tricked, but it also helps inform the generator about the identifiable mistakes in the generated images. At the start, the generator produces confused, three-eyed monsters that look nothing like a Rembrandt portrait. The discriminator is easily able to distinguish the muddled messes from the real paintings. As training progresses, information flows back from the discriminator, and the generator uses it to improve. By the end of training, the generator is able to produce convincing fakes, and the discriminator no longer is able to tell which is which.

Note that "Discriminator wins" or "Generator wins" shouldn't be taken literally—there's no explicit tournament between the two. However, both networks are trained based on the outcome of the other network, which drives the optimization of the parameters of each network.

This technique has proven itself able to lead to generators that produce realistic images from nothing but noise and a conditioning signal, like an attribute (for example, for faces: young, female, glasses on) or another image. In other words, a well-trained generator learns a plausible model for generating images that look real even when examined by humans.

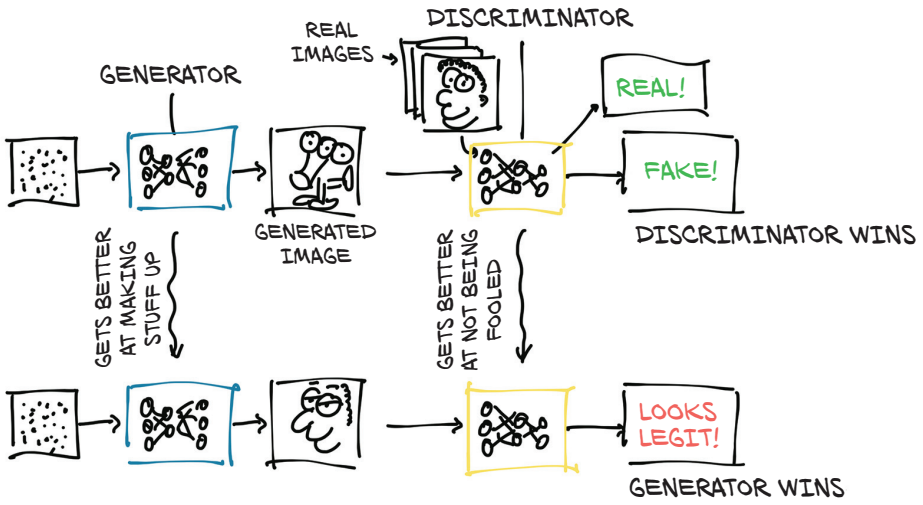


Figure 2.5 Concept of a GAN game

2.2.2 CycleGAN

An interesting evolution of this concept is the CycleGAN. A CycleGAN can turn images of one domain into images of another domain (and back), without the need for us to explicitly provide matching pairs in the training set.

In figure 2.6, we have a CycleGAN workflow for the task of turning a photo of a horse into a zebra, and vice versa. Note that there are two separate generator networks, as well as two distinct discriminators.

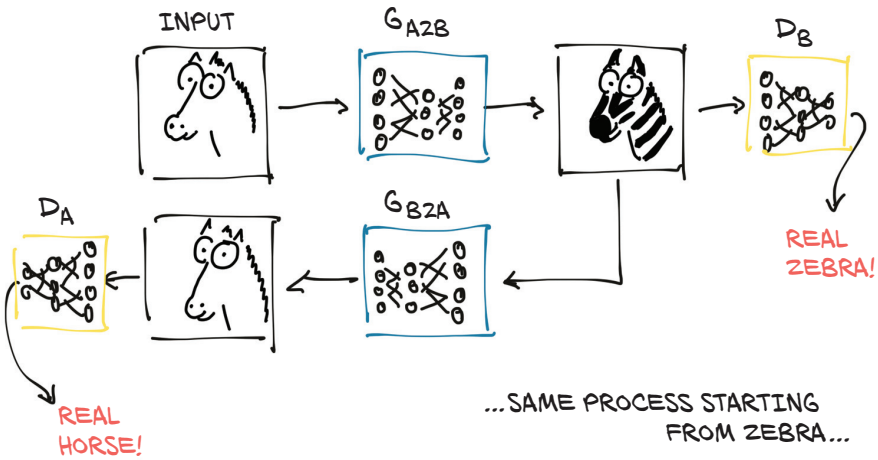


Figure 2.6 A CycleGAN trained to the point that it can fool both discriminator networks

As the figure shows, the first generator learns to produce an image conforming to a target distribution (zebras, in this case) starting from an image belonging to a different distribution (horses), so that the discriminator can't tell if the image produced from a horse photo is actually a genuine picture of a zebra or not. At the same time—and here's where the *Cycle* prefix in the acronym comes in—the resulting fake zebra is sent through a different generator going the other way (zebra to horse, in our case), to be judged by another discriminator on the other side. Creating such a cycle stabilizes the training process considerably, which addresses one of the original issues with GANs.

The fun part is that at this point, we don't need matched horse/zebra pairs as ground truths (good luck getting them to match poses!). It's enough to start from a collection of unrelated horse images and zebra photos for the generators to learn their task, going beyond a purely supervised setting. The implications of this model go even further than this: the generator learns how to selectively change the appearance of objects in the scene without supervision about what's what. There's no signal indicating that manes are manes and legs are legs, but they get translated to something that lines up with the anatomy of the other animal.

2.2.3 A network that turns horses into zebras

We can play with this model right now. The CycleGAN network has been trained on a dataset of (unrelated) horse images and zebra images extracted from the ImageNet dataset. The network learns to take an image of one or more horses and turn them all into zebras, leaving the rest of the image as unmodified as possible. While humankind hasn't held its breath over the last few thousand years for a tool that turn horses into zebras, this task showcases the ability of these architectures to model complex real-world processes with distant supervision. While they have their limits, there are hints that in the near future we won't be able to tell real from fake in a live video feed, which opens a can of worms that we'll duly close right now.

Playing with a pretrained CycleGAN will give us the opportunity to take a step closer and look at how a network—a generator, in this case—is implemented. We'll use our old friend ResNet. We'll define a `ResNetGenerator` class offscreen. The code is in the first cell of the 3_cyclegan.ipynb file, but the implementation isn't relevant right now, and it's too complex to follow until we've gotten a lot more PyTorch experience. Right now, we're focused on *what* it can do, rather than *how* it does it. Let's instantiate the class with default parameters (code/p1ch2/3_cyclegan.ipynb):

```
# In[2]:
netG = ResNetGenerator()
```

The `netG` model has been created, but it contains random weights. We mentioned earlier that we would run a generator model that had been pretrained on the horse2zebra dataset, whose training set contains two sets of 1068 and 1335 images of horses and zebras, respectively. The dataset be found at http://mng.bz/8pKP. The weights of the model have been saved in a .pth file, which is nothing but a `pickle` file of the model's

tensor parameters. We can load those into `ResNetGenerator` using the model's `load_state_dict` method:

```
# In[3]:
model_path = '../data/p1ch2/horse2zebra_0.4.0.pth'
model_data = torch.load(model_path)
netG.load_state_dict(model_data)
```

At this point, `netG` has acquired all the knowledge it achieved during training. Note that this is fully equivalent to what happened when we loaded `resnet101` from `torchvision` in section 2.1.3; but the `torchvision.resnet101` function hid the loading from us.

Let's put the network in `eval` mode, as we did for `resnet101`:

```
# In[4]:
netG.eval()

# Out[4]:
ResNetGenerator(
  (model): Sequential(
...
  )
)
```

Printing out the model as we did earlier, we can appreciate that it's actually pretty condensed, considering what it does. It takes an image, recognizes one or more horses in it by looking at pixels, and individually modifies the values of those pixels so that what comes out looks like a credible zebra. We won't recognize anything zebra-like in the printout (or in the source code, for that matter): that's because there's nothing zebra-like in there. The network is a scaffold—the juice is in the weights.

We're ready to load a random image of a horse and see what our generator produces. First, we need to import `PIL` and `torchvision`:

```
# In[5]:
from PIL import Image
from torchvision import transforms
```

Then we define a few input transformations to make sure data enters the network with the right shape and size:

```
# In[6]:
preprocess = transforms.Compose([transforms.Resize(256),
                                 transforms.ToTensor()])
```

Let's open a horse file (see figure 2.7):

```
# In[7]:
img = Image.open("../data/p1ch2/horse.jpg")
img
```

Figure 2.7 A man riding a horse. The horse is not having it.

OK, there's a dude on the horse. (Not for long, judging by the picture.) Anyhow, let's pass it through preprocessing and turn it into a properly shaped variable:

```
# In[8]:
img_t = preprocess(img)
batch_t = torch.unsqueeze(img_t, 0)
```

We shouldn't worry about the details right now. The important thing is that we follow from a distance. At this point, `batch_t` can be sent to our model:

```
# In[9]:
batch_out = netG(batch_t)
```

`batch_out` is now the output of the generator, which we can convert back to an image:

```
# In[10]:
out_t = (batch_out.data.squeeze() + 1.0) / 2.0
out_img = transforms.ToPILImage()(out_t)
# out_img.save('../data/p1ch2/zebra.jpg')
out_img

# Out[10]:
<PIL.Image.Image image mode=RGB size=316x256 at 0x23B24634F98>
```

Oh, man. Who rides a zebra that way? The resulting image (figure 2.8) is not perfect, but consider that it is a bit unusual for the network to find someone (sort of) riding on top of a horse. It bears repeating that the learning process has not passed through direct supervision, where humans have delineated tens of thousands of horses or manually Photoshopped thousands of zebra stripes. The generator has learned to produce an image that would fool the discriminator into thinking that was a zebra, and there was nothing fishy about the image (clearly the discriminator has never been to a rodeo).

Figure 2.8 A man riding a zebra. The zebra is not having it.

Many other fun generators have been developed using adversarial training or other approaches. Some of them are capable of creating credible human faces of nonexistent individuals; others can translate sketches into real-looking pictures of imaginary landscapes. Generative models are also being explored for producing real-sounding audio, credible text, and enjoyable music. It is likely that these models will be the basis of future tools that support the creative process.

On a serious note, it's hard to overstate the implications of this kind of work. Tools like the one we just downloaded are only going to become higher quality and more ubiquitous. Face-swapping technology, in particular, has gotten considerable media attention. Searching for "deep fakes" will turn up a plethora of example content[1] (though we must note that there is a nontrivial amount of not-safe-for-work content labeled as such; as with everything on the internet, click carefully).

So far, we've had a chance to play with a model that sees into images and a model that generates new images. We'll end our tour with a model that involves one more, fundamental ingredient: natural language.

2.3 A pretrained network that describes scenes

In order to get firsthand experience with a model involving natural language, we will use a pretrained image-captioning model, generously provided by Ruotian Luo.[2] It is an implementation of the NeuralTalk2 model by Andrej Karpathy. When presented with a natural image, this kind of model generates a caption in English that describes the scene, as shown in figure 2.9. The model is trained on a large dataset of images

[1] A relevant example is described in the Vox article "Jordan Peele's simulated Obama PSA is a double-edged warning against fake news," by Aja Romano; http://mng.bz/dxBz (warning: coarse language).

[2] We maintain a clone of the code at https://github.com/deep-learning-with-pytorch/ImageCaptioning.pytorch.

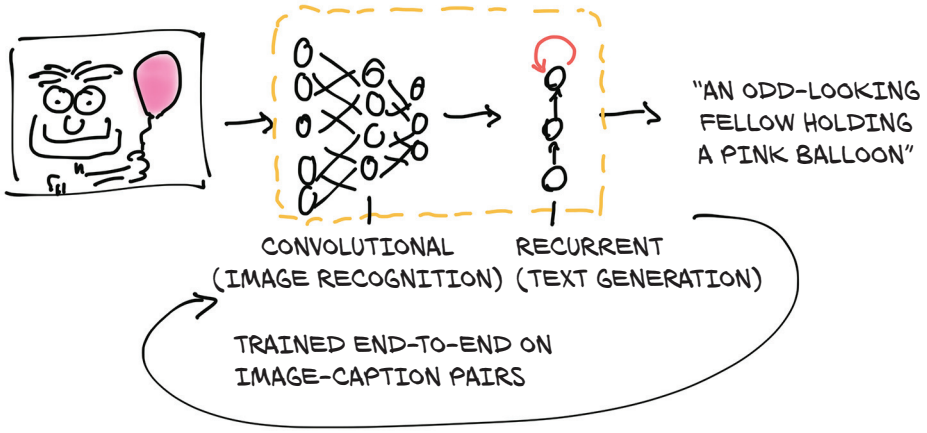


Figure 2.9 Concept of a captioning model

along with a paired sentence description: for example, "A Tabby cat is leaning on a wooden table, with one paw on a laser mouse and the other on a black laptop."[3]

This captioning model has two connected halves. The first half of the model is a network that learns to generate "descriptive" numerical representations of the scene (Tabby cat, laser mouse, paw), which are then taken as input to the second half. That second half is a *recurrent neural network* that generates a coherent sentence by putting those numerical descriptions together. The two halves of the model are trained together on image-caption pairs.

The second half of the model is called *recurrent* because it generates its outputs (individual words) in subsequent forward passes, where the input to each forward pass includes the outputs of the previous forward pass. This generates a dependency of the next word on words that were generated earlier, as we would expect when dealing with sentences or, in general, with sequences.

2.3.1 NeuralTalk2

The NeuralTalk2 model can be found at https://github.com/deep-learning-with-pytorch/ImageCaptioning.pytorch. We can place a set of images in the `data` directory and run the following script:

```
python eval.py --model ./data/FC/fc-model.pth
➥ --infos_path ./data/FC/fc-infos.pkl --image_folder ./data
```

Let's try it with our horse.jpg image. It says, "A person riding a horse on a beach." Quite appropriate.

[3] Andrej Karpathy and Li Fei-Fei, "Deep Visual-Semantic Alignments for Generating Image Descriptions," https://cs.stanford.edu/people/karpathy/cvpr2015.pdf.

Now, just for fun, let's see if our CycleGAN can also fool this NeuralTalk2 model. Let's add the zebra.jpg image in the data folder and rerun the model: "A group of zebras are standing in a field." Well, it got the animal right, but it saw more than one zebra in the image. Certainly this is not a pose that the network has ever seen a zebra in, nor has it ever seen a rider on a zebra (with some spurious zebra patterns). In addition, it is very likely that zebras are depicted in groups in the training dataset, so there might be some bias that we could investigate. The captioning network hasn't described the rider, either. Again, it's probably for the same reason: the network wasn't shown a rider on a zebra in the training dataset. In any case, this is an impressive feat: we generated a fake image with an impossible situation, and the captioning network was flexible enough to get the subject right.

We'd like to stress that something like this, which would have been extremely hard to achieve before the advent of deep learning, can be obtained with under a thousand lines of code, with a general-purpose architecture that knows nothing about horses or zebras, and a corpus of images and their descriptions (the MS COCO dataset, in this case). No hardcoded criterion or grammar—everything, including the sentence, emerges from patterns in the data.

The network architecture in this last case was, in a way, more complex than the ones we saw earlier, as it includes two networks. One is recurrent, but it was built out of the same building blocks, all of which are provided by PyTorch.

At the time of this writing, models such as these exist more as applied research or novelty projects, rather than something that has a well-defined, concrete use. The results, while promising, just aren't good enough to use … yet. With time (and additional training data), we should expect this class of models to be able to describe the world to people with vision impairment, transcribe scenes from video, and perform other similar tasks.

2.4 Torch Hub

Pretrained models have been published since the early days of deep learning, but until PyTorch 1.0, there was no way to ensure that users would have a uniform interface to get them. TorchVision was a good example of a clean interface, as we saw earlier in this chapter; but other authors, as we have seen for CycleGAN and NeuralTalk2, chose different designs.

PyTorch 1.0 saw the introduction of Torch Hub, which is a mechanism through which authors can publish a model on GitHub, with or without pretrained weights, and expose it through an interface that PyTorch understands. This makes loading a pretrained model from a third party as easy as loading a TorchVision model.

All it takes for an author to publish a model through the Torch Hub mechanism is to place a file named hubconf.py in the root directory of the GitHub repository. The file has a very simple structure:

```
# Optional list of modules the code depends on
dependencies = ['torch', 'math']

def some_entry_fn(*args, **kwargs):
    model = build_some_model(*args, **kwargs)
    return model

def another_entry_fn(*args, **kwargs):
    model = build_another_model(*args, **kwargs)
    return model
```

One or more functions to be exposed to users as entry points for the repository. These functions should initialize models according to the arguments and return them.

In our quest for interesting pretrained models, we can now search for GitHub repositories that include hubconf.py, and we'll know right away that we can load them using the torch.hub module. Let's see how this is done in practice. To do that, we'll go back to TorchVision, because it provides a clean example of how to interact with Torch Hub.

Let's visit https://github.com/pytorch/vision and notice that it contains a hubconf.py file. Great, that checks. The first thing to do is to look in that file to see the entry points for the repo—we'll need to specify them later. In the case of TorchVision, there are two: `resnet18` and `resnet50`. We already know what these do: they return an 18-layer and a 50-layer ResNet model, respectively. We also see that the entry-point functions include a `pretrained` keyword argument. If `True`, the returned models will be initialized with weights learned from ImageNet, as we saw earlier in the chapter.

Now we know the repo, the entry points, and one interesting keyword argument. That's about all we need to load the model using torch.hub, without even cloning the repo. That's right, PyTorch will handle that for us:

```
import torch
from torch import hub

resnet18_model = hub.load('pytorch/vision:master',
                          'resnet18',
                          pretrained=True)
```

Name and branch of the GitHub repo

Name of the entry-point function

Keyword argument

This manages to download a snapshot of the master branch of the pytorch/vision repo, along with the weights, to a local directory (defaults to .torch/hub in our home directory) and run the `resnet18` entry-point function, which returns the instantiated model. Depending on the environment, Python may complain that there's a module missing, like `PIL`. Torch Hub won't install missing dependencies, but it will report them to us so that we can take action.

At this point, we can invoke the returned model with proper arguments to run a forward pass on it, the same way we did earlier. The nice part is that now every model published through this mechanism will be accessible to us using the same modalities, well beyond vision.

Note that entry points are supposed to return models; but, strictly speaking, they are not forced to. For instance, we could have an entry point for transforming inputs and another one for turning the output probabilities into a text label. Or we could have an entry point for just the model, and another that includes the model along with the pre- and postprocessing steps. By leaving these options open, the PyTorch developers have provided the community with just enough standardization and a lot of flexibility. We'll see what patterns will emerge from this opportunity.

Torch Hub is quite new at the time of writing, and there are only a few models published this way. We can get at them by Googling "github.com hubconf.py." Hopefully the list will grow in the future, as more authors share their models through this channel.

2.5 Conclusion

We hope this was a fun chapter. We took some time to play with models created with PyTorch, which were optimized to carry out specific tasks. In fact, the more enterprising of us could already put one of these models behind a web server and start a business, sharing the profits with the original authors![4] Once we learn how these models are built, we will also be able to use the knowledge we gained here to download a pretrained model and quickly fine-tune it on a slightly different task.

We will also see how building models that deal with different problems on different kinds of data can be done using the same building blocks. One thing that PyTorch does particularly right is providing those building blocks in the form of an essential toolset—PyTorch is not a very large library from an API perspective, especially when compared with other deep learning frameworks.

This book does not focus on going through the complete PyTorch API or reviewing deep learning architectures; rather, we will build hands-on knowledge of these building blocks. This way, you will be able to consume the excellent online documentation and repositories on top of a solid foundation.

Starting with the next chapter, we'll embark on a journey that will enable us to teach our computer skills like those described in this chapter from scratch, using PyTorch. We'll also learn that starting from a pretrained network and fine-tuning it on new data, without starting from scratch, is an effective way to solve problems when the data points we have are not particularly numerous. This is one further reason pretrained networks are an important tool for deep learning practitioners to have. Time to learn about the first fundamental building block: tensors.

[4] Contact the publisher for franchise opportunities!

2.6 Exercises

1. Feed the image of the golden retriever into the horse-to-zebra model.
   a. What do you need to do to the image to prepare it?
   b. What does the output look like?
2. Search GitHub for projects that provide a hubconf.py file.
   a. How many repositories are returned?
   b. Find an interesting-looking project with a hubconf.py. Can you understand the purpose of the project from the documentation?
   c. Bookmark the project, and come back after you've finished this book. Can you understand the implementation?

2.7 Summary

- A pretrained network is a model that has already been trained on a dataset. Such networks can typically produce useful results immediately after loading the network parameters.
- By knowing how to use a pretrained model, we can integrate a neural network into a project without having to design or train it.
- AlexNet and ResNet are two deep convolutional networks that set new benchmarks for image recognition in the years they were released.
- Generative adversarial networks (GANs) have two parts—the generator and the discriminator—that work together to produce output indistinguishable from authentic items.
- CycleGAN uses an architecture that supports converting back and forth between two different classes of images.
- NeuralTalk2 uses a hybrid model architecture to consume an image and produce a text description of the image.
- Torch Hub is a standardized way to load models and weights from any project with an appropriate hubconf.py file.

3 It starts with a tensor

This chapter covers

- Understanding tensors, the basic data structure in PyTorch
- Indexing and operating on tensors
- Interoperating with NumPy multidimensional arrays
- Moving computations to the GPU for speed

In the previous chapter, we took a tour of some of the many applications that deep learning enables. They invariably consisted of taking data in some form, like images or text, and producing data in another form, like labels, numbers, or more images or text. Viewed from this angle, deep learning really consists of building a system that can transform data from one representation to another. This transformation is driven by extracting commonalities from a series of examples that demonstrate the desired mapping. For example, the system might note the general shape of a dog and the typical colors of a golden retriever. By combining the two image properties, the system can correctly map images with a given shape and color to the golden retriever label, instead of a black lab (or a tawny tomcat, for that matter). The resulting system can consume broad swaths of similar inputs and produce meaningful output for those inputs.

The process begins by converting our input into floating-point numbers. We will cover converting image pixels to numbers, as we see in the first step of figure 3.1, in chapter 4 (along with many other types of data). But before we can get to that, in this chapter, we learn how to deal with all the floating-point numbers in PyTorch by using tensors.

3.1 The world as floating-point numbers

Since floating-point numbers are the way a network deals with information, we need a way to encode real-world data of the kind we want to process into something digestible by a network and then decode the output back to something we can understand and use for our purpose.

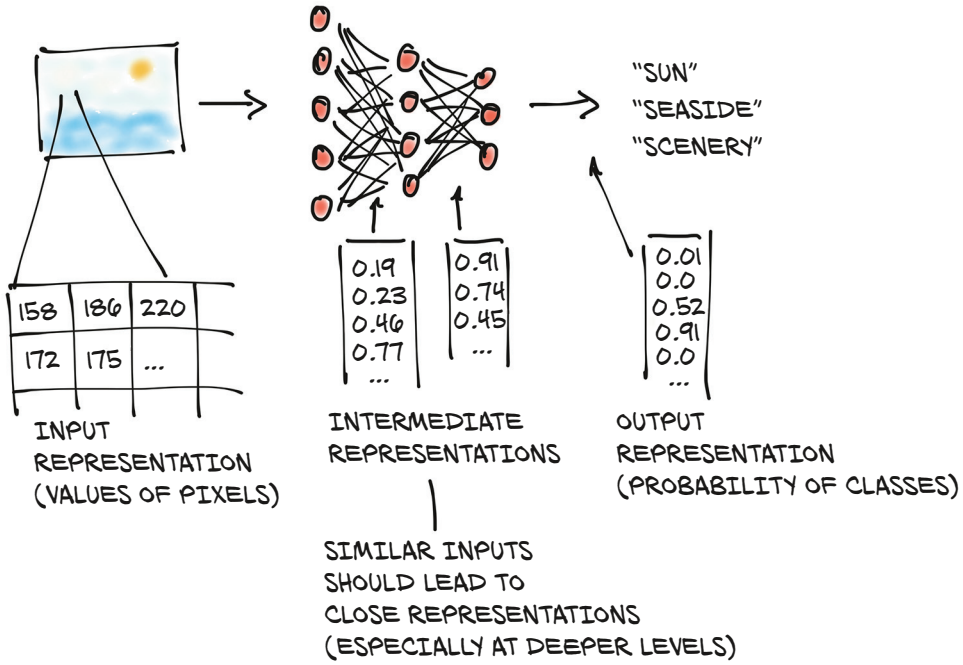


Figure 3.1 A deep neural network learns how to transform an input representation to an output representation. (Note: The numbers of neurons and outputs are not to scale.)

A deep neural network typically learns the transformation from one form of data to another in stages, which means the partially transformed data between each stage can be thought of as a sequence of intermediate representations. For image recognition, early representations can be things such as edge detection or certain textures like fur. Deeper representations can capture more complex structures like ears, noses, or eyes.

In general, such intermediate representations are collections of floating-point numbers that characterize the input and capture the data's structure in a way that is instrumental for describing how inputs are mapped to the outputs of the neural network. Such characterization is specific to the task at hand and is learned from relevant

examples. These collections of floating-point numbers and their manipulation are at the heart of modern AI—we will see several examples of this throughout the book.

It's important to keep in mind that these intermediate representations (like those shown in the second step of figure 3.1) are the results of combining the input with the weights of the previous layer of neurons. Each intermediate representation is unique to the inputs that preceeded it.

Before we can begin the process of converting our data to floating-point input, we must first have a solid understanding of how PyTorch handles and stores data—as input, as intermediate representations, and as output. This chapter will be devoted to precisely that.

To this end, PyTorch introduces a fundamental data structure: the *tensor*. We already bumped into tensors in chapter 2, when we ran inference on pretrained networks. For those who come from mathematics, physics, or engineering, the term *tensor* comes bundled with the notion of spaces, reference systems, and transformations between them. For better or worse, those notions do not apply here. In the context of deep learning, tensors refer to the generalization of vectors and matrices to an arbitrary number of dimensions, as we can see in figure 3.2. Another name for the same concept is *multidimensional array*. The dimensionality of a tensor coincides with the number of indexes used to refer to scalar values within the tensor.

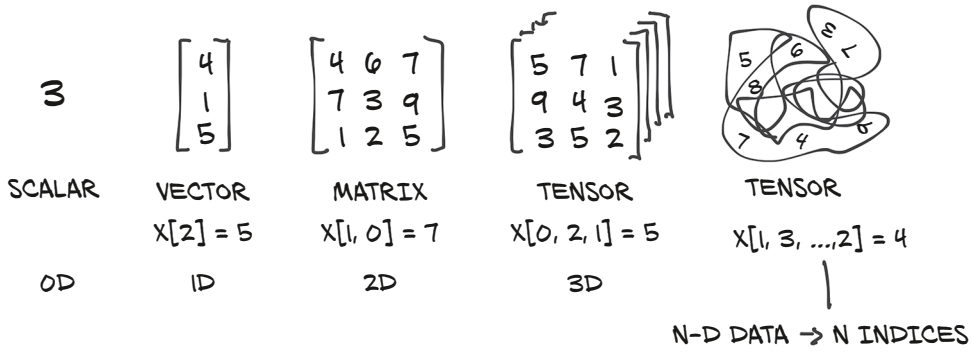


Figure 3.2 Tensors are the building blocks for representing data in PyTorch.

PyTorch is not the only library that deals with multidimensional arrays. NumPy is by far the most popular multidimensional array library, to the point that it has now arguably become the *lingua franca* of data science. PyTorch features seamless interoperability with NumPy, which brings with it first-class integration with the rest of the scientific libraries in Python, such as SciPy (www.scipy.org), Scikit-learn (https://scikit-learn.org), and Pandas (https://pandas.pydata.org).

Compared to NumPy arrays, PyTorch tensors have a few superpowers, such as the ability to perform very fast operations on graphical processing units (GPUs), distribute operations on multiple devices or machines, and keep track of the graph of

computations that created them. These are all important features when implementing a modern deep learning library.

We'll start this chapter by introducing PyTorch tensors, covering the basics in order to set things in motion for our work in the rest of the book. First and foremost, we'll learn how to manipulate tensors using the PyTorch tensor library. This includes things like how the data is stored in memory, how certain operations can be performed on arbitrarily large tensors in constant time, and the aforementioned NumPy interoperability and GPU acceleration. Understanding the capabilities and API of tensors is important if they're to become go-to tools in our programming toolbox. In the next chapter, we'll put this knowledge to good use and learn how to represent several different kinds of data in a way that enables learning with neural networks.

3.2 Tensors: Multidimensional arrays

We have already learned that tensors are the fundamental data structure in PyTorch. A tensor is an array: that is, a data structure that stores a collection of numbers that are accessible individually using an index, and that can be indexed with multiple indices.

3.2.1 From Python lists to PyTorch tensors

Let's see `list` indexing in action so we can compare it to tensor indexing. Take a list of three numbers in Python (.code/p1ch3/1_tensors.ipynb):

```
# In[1]:
a = [1.0, 2.0, 1.0]
```

We can access the first element of the list using the corresponding zero-based index:

```
# In[2]:
a[0]

# Out[2]:
1.0

# In[3]:
a[2] = 3.0
a

# Out[3]:
[1.0, 2.0, 3.0]
```

It is not unusual for simple Python programs dealing with vectors of numbers, such as the coordinates of a 2D line, to use Python lists to store the vectors. As we will see in the following chapter, using the more efficient tensor data structure, many types of data—from images to time series, and even sentences—can be represented. By defining operations over tensors, some of which we'll explore in this chapter, we can slice and manipulate data expressively and efficiently at the same time, even from a high-level (and not particularly fast) language such as Python.

3.2.2 Constructing our first tensors

Let's construct our first PyTorch tensor and see what it looks like. It won't be a particularly meaningful tensor for now, just three ones in a column:

```
# In[4]:
import torch
a = torch.ones(3)
a

# Out[4]:
tensor([1., 1., 1.])

# In[5]:
a[1]

# Out[5]:
tensor(1.)

# In[6]:
float(a[1])

# Out[6]:
1.0

# In[7]:
a[2] = 2.0
a

# Out[7]:
tensor([1., 1., 2.])
```

Imports the torch module

Creates a one-dimensional tensor of size 3 filled with 1s

After importing the `torch` module, we call a function that creates a (one-dimensional) tensor of size 3 filled with the value `1.0`. We can access an element using its zero-based index or assign a new value to it. Although on the surface this example doesn't differ much from a list of number objects, under the hood things are completely different.

3.2.3 The essence of tensors

Python lists or tuples of numbers are collections of Python objects that are individually allocated in memory, as shown on the left in figure 3.3. PyTorch tensors or NumPy arrays, on the other hand, are views over (typically) contiguous memory blocks containing *unboxed* C numeric types rather than Python objects. Each element is a 32-bit (4-byte) `float` in this case, as we can see on the right side of figure 3.3. This means storing a 1D tensor of 1,000,000 float numbers will require exactly 4,000,000 contiguous bytes, plus a small overhead for the metadata (such as dimensions and numeric type).

Say we have a list of coordinates we'd like to use to represent a geometrical object: perhaps a 2D triangle with vertices at coordinates (4, 1), (5, 3), and (2, 1). The example is not particularly pertinent to deep learning, but it's easy to follow. Instead of having coordinates as numbers in a Python list, as we did earlier, we can use a

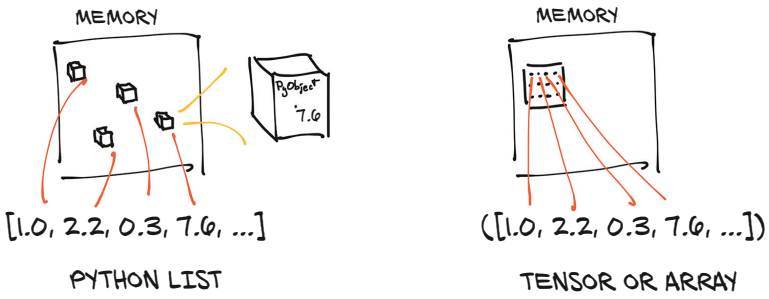


Figure 3.3 Python object (boxed) numeric values versus tensor (unboxed array) numeric values

one-dimensional tensor by storing *X*s in the even indices and *Y*s in the odd indices, like this:

```
# In[8]:
points = torch.zeros(6)
points[0] = 4.0
points[1] = 1.0
points[2] = 5.0
points[3] = 3.0
points[4] = 2.0
points[5] = 1.0
```

Using .zeros is just a way to get an appropriately sized array.

We overwrite those zeros with the values we actually want.

We can also pass a Python list to the constructor, to the same effect:

```
# In[9]:
points = torch.tensor([4.0, 1.0, 5.0, 3.0, 2.0, 1.0])
points

# Out[9]:
tensor([4., 1., 5., 3., 2., 1.])
```

To get the coordinates of the first point, we do the following:

```
# In[10]:
float(points[0]), float(points[1])

# Out[10]:
(4.0, 1.0)
```

This is OK, although it would be practical to have the first index refer to individual 2D points rather than point coordinates. For this, we can use a 2D tensor:

```
# In[11]:
points = torch.tensor([[4.0, 1.0], [5.0, 3.0], [2.0, 1.0]])
points
```

```
# Out[11]:
tensor([[4., 1.],
        [5., 3.],
        [2., 1.]])
```

Here, we pass a list of lists to the constructor. We can ask the tensor about its shape:

```
# In[12]:
points.shape

# Out[12]:
torch.Size([3, 2])
```

This informs us about the size of the tensor along each dimension. We could also use `zeros` or `ones` to initialize the tensor, providing the size as a tuple:

```
# In[13]:
points = torch.zeros(3, 2)
points

# Out[13]:
tensor([[0., 0.],
        [0., 0.],
        [0., 0.]])
```

Now we can access an individual element in the tensor using two indices:

```
# In[14]:
points = torch.tensor([[4.0, 1.0], [5.0, 3.0], [2.0, 1.0]])
points

# Out[14]:
tensor([[4., 1.],
        [5., 3.],
        [2., 1.]])

# In[15]:
points[0, 1]

# Out[15]:
tensor(1.)
```

This returns the *Y*-coordinate of the zeroth point in our dataset. We can also access the first element in the tensor as we did before to get the 2D coordinates of the first point:

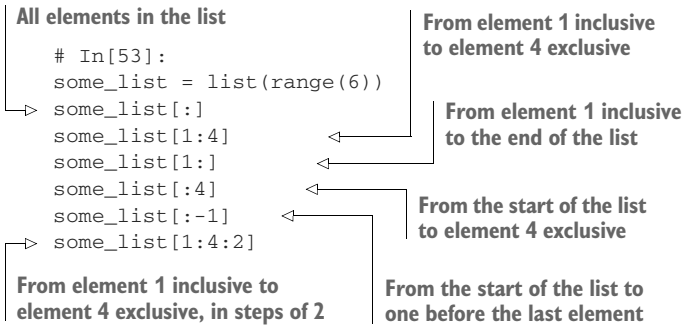
```
# In[16]:
points[0]

# Out[16]:
tensor([4., 1.])
```

The output is another tensor that presents a different *view* of the same underlying data. The new tensor is a 1D tensor of size 2, referencing the values of the first row in the `points` tensor. Does this mean a new chunk of memory was allocated, values were copied into it, and the new memory was returned wrapped in a new tensor object? No, because that would be very inefficient, especially if we had millions of points. We'll revisit how tensors are stored later in this chapter when we cover views of tensors in section 3.7.

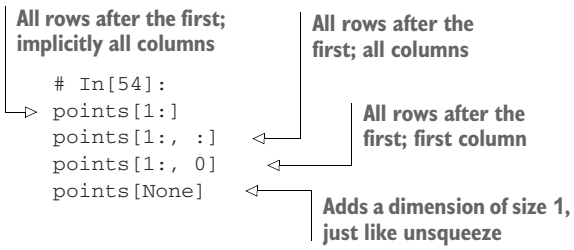
3.3 Indexing tensors

What if we need to obtain a tensor containing all points but the first? That's easy using range indexing notation, which also applies to standard Python lists. Here's a reminder:




```
# In[53]:
some_list = list(range(6))
some_list[:]
some_list[1:4]
some_list[1:]
some_list[:4]
some_list[:-1]
some_list[1:4:2]
```

To achieve our goal, we can use the same notation for PyTorch tensors, with the added benefit that, just as in NumPy and other Python scientific libraries, we can use range indexing for each of the tensor's dimensions:




```
# In[54]:
points[1:]
points[1:, :]
points[1:, 0]
points[None]
```

In addition to using ranges, PyTorch features a powerful form of indexing, called *advanced indexing*, which we will look at in the next chapter.

3.4 Named tensors

The dimensions (or axes) of our tensors usually index something like pixel locations or color channels. This means when we want to index into a tensor, we need to remember the ordering of the dimensions and write our indexing accordingly. As data is transformed through multiple tensors, keeping track of which dimension contains what data can be error-prone.

To make things concrete, imagine that we have a 3D tensor like `img_t` from section 2.1.4 (we will use dummy data for simplicity here), and we want to convert it to grayscale. We looked up typical weights for the colors to derive a single brightness value:[1]

```
# In[2]:
img_t = torch.randn(3, 5, 5) # shape [channels, rows, columns]
weights = torch.tensor([0.2126, 0.7152, 0.0722])
```

We also often want our code to generalize—for example, from grayscale images represented as 2D tensors with height and width dimensions to color images adding a third channel dimension (as in RGB), or from a single image to a batch of images. In section 2.1.4, we introduced an additional batch dimension in `batch_t`; here we pretend to have a batch of 2:

```
# In[3]:
batch_t = torch.randn(2, 3, 5, 5) # shape [batch, channels, rows, columns]
```

So sometimes the RGB channels are in dimension 0, and sometimes they are in dimension 1. But we can generalize by counting from the end: they are always in dimension –3, the third from the end. The lazy, unweighted mean can thus be written as follows:

```
# In[4]:
img_gray_naive = img_t.mean(-3)
batch_gray_naive = batch_t.mean(-3)
img_gray_naive.shape, batch_gray_naive.shape

# Out[4]:
(torch.Size([5, 5]), torch.Size([2, 5, 5]))
```

But now we have the weight, too. PyTorch will allow us to multiply things that are the same shape, as well as shapes where one operand is of size 1 in a given dimension. It also appends leading dimensions of size 1 automatically. This is a feature called *broadcasting*. `batch_t` of shape (2, 3, 5, 5) is multiplied by `unsqueezed_weights` of shape (3, 1, 1), resulting in a tensor of shape (2, 3, 5, 5), from which we can then sum the third dimension from the end (the three channels):

```
# In[5]:
unsqueezed_weights = weights.unsqueeze(-1).unsqueeze_(-1)
img_weights = (img_t * unsqueezed_weights)
batch_weights = (batch_t * unsqueezed_weights)
img_gray_weighted = img_weights.sum(-3)
batch_gray_weighted = batch_weights.sum(-3)
batch_weights.shape, batch_t.shape, unsqueezed_weights.shape

# Out[5]:
(torch.Size([2, 3, 5, 5]), torch.Size([2, 3, 5, 5]), torch.Size([3, 1, 1]))
```

[1] As perception is not trivial to norm, people have come up with many weights. For example, see https://en.wikipedia.org/wiki/Luma_(video).

Because this gets messy quickly—and for the sake of efficiency—the PyTorch function `einsum` (adapted from NumPy) specifies an indexing mini-language[2] giving index names to dimensions for sums of such products. As often in Python, broadcasting—a form of summarizing unnamed things—is done using three dots `'...'`; but don't worry too much about `einsum`, because we will not use it in the following:

```
# In[6]:
img_gray_weighted_fancy = torch.einsum('...chw,c->...hw', img_t, weights)
batch_gray_weighted_fancy = torch.einsum('...chw,c->...hw', batch_t, weights)
batch_gray_weighted_fancy.shape

# Out[6]:
torch.Size([2, 5, 5])
```

As we can see, there is quite a lot of bookkeeping involved. This is error-prone, especially when the locations where tensors are created and used are far apart in our code. This has caught the eye of practitioners, and so it has been suggested[3] that the dimension be given a name instead.

PyTorch 1.3 added *named tensors* as an experimental feature (see https://pytorch.org/tutorials/intermediate/named_tensor_tutorial.html and https://pytorch.org/docs/stable/named_tensor.html). Tensor factory functions such as `tensor` and `rand` take a `names` argument. The names should be a sequence of strings:

```
# In[7]:
weights_named = torch.tensor([0.2126, 0.7152, 0.0722], names=['channels'])
weights_named

# Out[7]:
tensor([0.2126, 0.7152, 0.0722], names=('channels',))
```

When we already have a tensor and want to add names (but not change existing ones), we can call the method `refine_names` on it. Similar to indexing, the ellipsis (…) allows you to leave out any number of dimensions. With the `rename` sibling method, you can also overwrite or drop (by passing in `None`) existing names:

```
# In[8]:
img_named =  img_t.refine_names(..., 'channels', 'rows', 'columns')
batch_named = batch_t.refine_names(..., 'channels', 'rows', 'columns')
print("img named:", img_named.shape, img_named.names)
print("batch named:", batch_named.shape, batch_named.names)

# Out[8]:
img named: torch.Size([3, 5, 5]) ('channels', 'rows', 'columns')
batch named: torch.Size([2, 3, 5, 5]) (None, 'channels', 'rows', 'columns')
```

---

[2] Tim Rocktäschel's blog post "Einsum is All You Need—Einstein Summation in Deep Learning" (https://rockt.github.io/2018/04/30/einsum) gives a good overview.

[3] See Sasha Rush, "Tensor Considered Harmful," Harvardnlp, http://nlp.seas.harvard.edu/NamedTensor.

For operations with two inputs, in addition to the usual dimension checks—whether sizes are the same, or if one is 1 and can be broadcast to the other—PyTorch will now check the names for us. So far, it does not automatically align dimensions, so we need to do this explicitly. The method `align_as` returns a tensor with missing dimensions added and existing ones permuted to the right order:

```
# In[9]:
weights_aligned = weights_named.align_as(img_named)
weights_aligned.shape, weights_aligned.names

# Out[9]:
(torch.Size([3, 1, 1]), ('channels', 'rows', 'columns'))
```

Functions accepting dimension arguments, like `sum`, also take named dimensions:

```
# In[10]:
gray_named = (img_named * weights_aligned).sum('channels')
gray_named.shape, gray_named.names

# Out[10]:
(torch.Size([5, 5]), ('rows', 'columns'))
```

If we try to combine dimensions with different names, we get an error:

```
gray_named = (img_named[..., :3] * weights_named).sum('channels')

RuntimeError: Error when
 attempting to broadcast dims ['channels', 'rows',
  'columns'] and dims ['channels']: dim 'columns' and dim 'channels'
  are at the same position from the right but do not match.
```

If we want to use tensors outside functions that operate on named tensors, we need to drop the names by renaming them to `None`. The following gets us back into the world of unnamed dimensions:

```
# In[12]:
gray_plain = gray_named.rename(None)
gray_plain.shape, gray_plain.names

# Out[12]:
(torch.Size([5, 5]), (None, None))
```

Given the experimental nature of this feature at the time of writing, and to avoid mucking around with indexing and alignment, we will stick to unnamed in the remainder of the book. Named tensors have the potential to eliminate many sources of alignment errors, which—if the PyTorch forum is any indication—can be a source of headaches. It will be interesting to see how widely they will be adopted.

3.5 Tensor element types

So far, we have covered the basics of how tensors work, but we have not yet touched on what kinds of numeric types we can store in a `Tensor`. As we hinted at in section 3.2, using the standard Python numeric types can be suboptimal for several reasons:

- *Numbers in Python are objects.* Whereas a floating-point number might require only, for instance, 32 bits to be represented on a computer, Python will convert it into a full-fledged Python object with reference counting, and so on. This operation, called *boxing*, is not a problem if we need to store a small number of numbers, but allocating millions gets very inefficient.
- *Lists in Python are meant for sequential collections of objects.* There are no operations defined for, say, efficiently taking the dot product of two vectors, or summing vectors together. Also, Python lists have no way of optimizing the layout of their contents in memory, as they are indexable collections of pointers to Python objects (of any kind, not just numbers). Finally, Python lists are one-dimensional, and although we can create lists of lists, this is again very inefficient.
- *The Python interpreter is slow compared to optimized, compiled code.* Performing mathematical operations on large collections of numerical data can be much faster using optimized code written in a compiled, low-level language like C.

For these reasons, data science libraries rely on NumPy or introduce dedicated data structures like PyTorch tensors, which provide efficient low-level implementations of numerical data structures and related operations on them, wrapped in a convenient high-level API. To enable this, the objects within a tensor must all be numbers of the same type, and PyTorch must keep track of this numeric type.

3.5.1 Specifying the numeric type with dtype

The `dtype` argument to tensor constructors (that is, functions like `tensor`, `zeros`, and `ones`) specifies the numerical data (d) type that will be contained in the tensor. The data type specifies the possible values the tensor can hold (integers versus floating-point numbers) and the number of bytes per value.[4] The `dtype` argument is deliberately similar to the standard NumPy argument of the same name. Here's a list of the possible values for the `dtype` argument:

- `torch.float32` or `torch.float`: 32-bit floating-point
- `torch.float64` or `torch.double`: 64-bit, double-precision floating-point
- `torch.float16` or `torch.half`: 16-bit, half-precision floating-point
- `torch.int8`: signed 8-bit integers
- `torch.uint8`: unsigned 8-bit integers
- `torch.int16` or `torch.short`: signed 16-bit integers
- `torch.int32` or `torch.int`: signed 32-bit integers
- `torch.int64` or `torch.long`: signed 64-bit integers
- `torch.bool`: Boolean

[4] And signed-ness, in the case of `uint8`.

The default data type for tensors is 32-bit floating-point.

3.5.2 A dtype for every occasion

As we will see in future chapters, computations happening in neural networks are typically executed with 32-bit floating-point precision. Higher precision, like 64-bit, will not buy improvements in the accuracy of a model and will require more memory and computing time. The 16-bit floating-point, half-precision data type is not present natively in standard CPUs, but it is offered on modern GPUs. It is possible to switch to half-precision to decrease the footprint of a neural network model if needed, with a minor impact on accuracy.

Tensors can be used as indexes in other tensors. In this case, PyTorch expects indexing tensors to have a 64-bit integer data type. Creating a tensor with integers as arguments, such as using `torch.tensor([2, 2])`, will create a 64-bit integer tensor by default. As such, we'll spend most of our time dealing with `float32` and `int64`.

Finally, predicates on tensors, such as `points > 1.0`, produce `bool` tensors indicating whether each individual element satisfies the condition. These are the numeric types in a nutshell.

3.5.3 Managing a tensor's dtype attribute

In order to allocate a tensor of the right numeric type, we can specify the proper `dtype` as an argument to the constructor. For example:

```
# In[47]:
double_points = torch.ones(10, 2, dtype=torch.double)
short_points = torch.tensor([[1, 2], [3, 4]], dtype=torch.short)
```

We can find out about the `dtype` for a tensor by accessing the corresponding attribute:

```
# In[48]:
short_points.dtype

# Out[48]:
torch.int16
```

We can also cast the output of a tensor creation function to the right type using the corresponding casting method, such as

```
# In[49]:
double_points = torch.zeros(10, 2).double()
short_points = torch.ones(10, 2).short()
```

or the more convenient `to` method:

```
# In[50]:
double_points = torch.zeros(10, 2).to(torch.double)
short_points = torch.ones(10, 2).to(dtype=torch.short)
```

Under the hood, `to` checks whether the conversion is necessary and, if so, does it. The `dtype`-named casting methods like `float` are shorthands for `to`, but the `to` method can take additional arguments that we'll discuss in section 3.9.

When mixing input types in operations, the inputs are converted to the larger type automatically. Thus, if we want 32-bit computation, we need to make sure all our inputs are (at most) 32-bit:

```
# In[51]:
points_64 = torch.rand(5, dtype=torch.double)
points_short = points_64.to(torch.short)
points_64 * points_short  # works from PyTorch 1.3 onwards

# Out[51]:
tensor([0., 0., 0., 0., 0.], dtype=torch.float64)
```

rand initializes the tensor elements to random numbers between 0 and 1.

3.6 The tensor API

At this point, we know what PyTorch tensors are and how they work under the hood. Before we wrap up, it is worth taking a look at the tensor operations that PyTorch offers. It would be of little use to list them all here. Instead, we're going to get a general feel for the API and establish a few directions on where to find things in the online documentation at http://pytorch.org/docs.

First, the vast majority of operations on and between tensors are available in the `torch` module and can also be called as methods of a tensor object. For instance, the `transpose` function we encountered earlier can be used from the `torch` module

```
# In[71]:
a = torch.ones(3, 2)
a_t = torch.transpose(a, 0, 1)

a.shape, a_t.shape

# Out[71]:
(torch.Size([3, 2]), torch.Size([2, 3]))
```

or as a method of the `a` tensor:

```
# In[72]:
a = torch.ones(3, 2)
a_t = a.transpose(0, 1)

a.shape, a_t.shape

# Out[72]:
(torch.Size([3, 2]), torch.Size([2, 3]))
```

There is no difference between the two forms; they can be used interchangeably.

We mentioned the online docs earlier (http://pytorch.org/docs). They are exhaustive and well organized, with the tensor operations divided into groups:

- *Creation ops*—Functions for constructing a tensor, like `ones` and `from_numpy`
- *Indexing, slicing, joining, mutating ops*—Functions for changing the shape, stride, or content of a tensor, like `transpose`
- *Math ops*—Functions for manipulating the content of the tensor through computations
  - *Pointwise ops*—Functions for obtaining a new tensor by applying a function to each element independently, like `abs` and `cos`
  - *Reduction ops*—Functions for computing aggregate values by iterating through tensors, like `mean`, `std`, and `norm`
  - *Comparison ops*—Functions for evaluating numerical predicates over tensors, like `equal` and `max`
  - *Spectral ops*—Functions for transforming in and operating in the frequency domain, like `stft` and `hamming_window`
  - *Other operations*—Special functions operating on vectors, like `cross`, or matrices, like `trace`
  - *BLAS and LAPACK operations*—Functions following the Basic Linear Algebra Subprograms (BLAS) specification for scalar, vector-vector, matrix-vector, and matrix-matrix operations
- *Random sampling*—Functions for generating values by drawing randomly from probability distributions, like `randn` and `normal`
- *Serialization*—Functions for saving and loading tensors, like `load` and `save`
- *Parallelism*—Functions for controlling the number of threads for parallel CPU execution, like `set_num_threads`

Take some time to play with the general tensor API. This chapter has provided all the prerequisites to enable this kind of interactive exploration. We will also encounter several of the tensor operations as we proceed with the book, starting in the next chapter.

3.7 Tensors: Scenic views of storage

It is time for us to look a bit closer at the implementation under the hood. Values in tensors are allocated in contiguous chunks of memory managed by `torch.Storage` instances. A storage is a one-dimensional array of numerical data: that is, a contiguous block of memory containing numbers of a given type, such as `float` (32 bits representing a floating-point number) or `int64` (64 bits representing an integer). A PyTorch `Tensor` instance is a view of such a `Storage` instance that is capable of indexing into that storage using an offset and per-dimension strides.[5]

Multiple tensors can index the same storage even if they index into the data differently. We can see an example of this in figure 3.4. In fact, when we requested `points[0]` in section 3.2, what we got back is another tensor that indexes the same

[5] `Storage` may not be directly accessible in future PyTorch releases, but what we show here still provides a good mental picture of how tensors work under the hood.

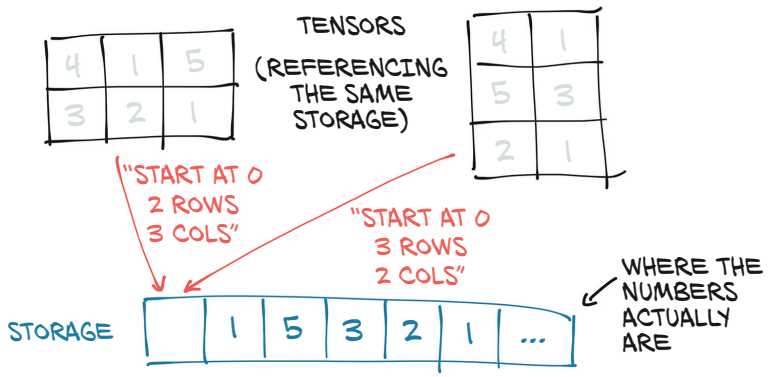


Figure 3.4 Tensors are views of a `Storage` instance.

storage as the `points` tensor—just not all of it, and with different dimensionality (1D versus 2D). The underlying memory is allocated only once, however, so creating alternate tensor-views of the data can be done quickly regardless of the size of the data managed by the `Storage` instance.

3.7.1 Indexing into storage

Let's see how indexing into the storage works in practice with our 2D points. The storage for a given tensor is accessible using the `.storage` property:

```
# In[17]:
points = torch.tensor([[4.0, 1.0], [5.0, 3.0], [2.0, 1.0]])
points.storage()

# Out[17]:
 4.0
 1.0
 5.0
 3.0
 2.0
 1.0
[torch.FloatStorage of size 6]
```

Even though the tensor reports itself as having three rows and two columns, the storage under the hood is a contiguous array of size 6. In this sense, the tensor just knows how to translate a pair of indices into a location in the storage.

We can also index into a storage manually. For instance:

```
# In[18]:
points_storage = points.storage()
points_storage[0]

# Out[18]:
4.0
```

```
# In[19]:
points.storage()[1]

# Out[19]:
1.0
```

We can't index a storage of a 2D tensor using two indices. The layout of a storage is always one-dimensional, regardless of the dimensionality of any and all tensors that might refer to it.

At this point, it shouldn't come as a surprise that changing the value of a storage leads to changing the content of its referring tensor:

```
# In[20]:
points = torch.tensor([[4.0, 1.0], [5.0, 3.0], [2.0, 1.0]])
points_storage = points.storage()
points_storage[0] = 2.0
points

# Out[20]:
tensor([[2., 1.],
        [5., 3.],
        [2., 1.]])
```

3.7.2 Modifying stored values: In-place operations

In addition to the operations on tensors introduced in the previous section, a small number of operations exist only as methods of the `Tensor` object. They are recognizable from a trailing underscore in their name, like `zero_`, which indicates that the method operates *in place* by modifying the input instead of creating a new output tensor and returning it. For instance, the `zero_` method zeros out all the elements of the input. Any method *without* the trailing underscore leaves the source tensor unchanged and instead returns a new tensor:

```
# In[73]:
a = torch.ones(3, 2)

# In[74]:
a.zero_()
a

# Out[74]:
tensor([[0., 0.],
        [0., 0.],
        [0., 0.]])
```

3.8 Tensor metadata: Size, offset, and stride

In order to index into a storage, tensors rely on a few pieces of information that, together with their storage, unequivocally define them: size, offset, and stride. How these interact is shown in figure 3.5. The size (or shape, in NumPy parlance) is a tuple

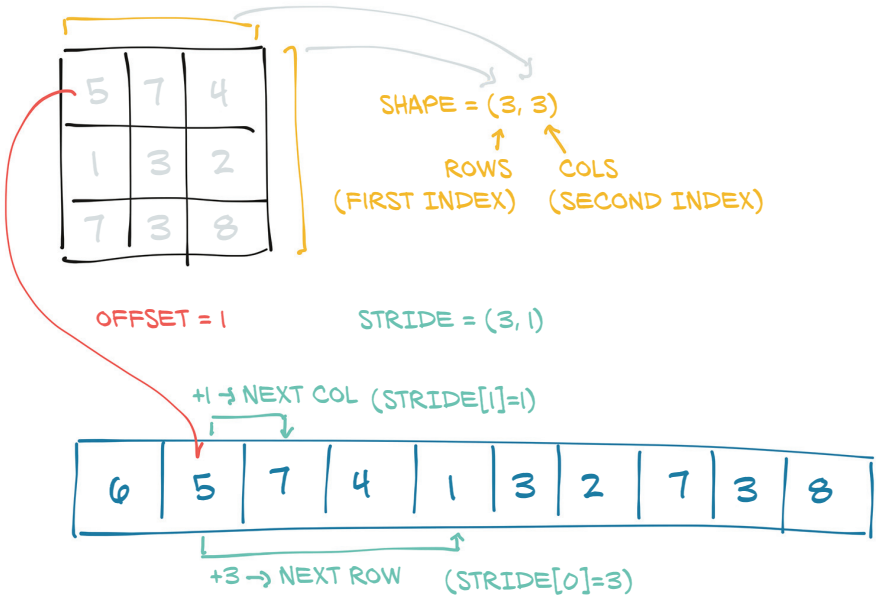


Figure 3.5 Relationship between a tensor's offset, size, and stride. Here the tensor is a view of a larger storage, like one that might have been allocated when creating a larger tensor.

indicating how many elements across each dimension the tensor represents. The storage offset is the index in the storage corresponding to the first element in the tensor. The stride is the number of elements in the storage that need to be skipped over to obtain the next element along each dimension.

3.8.1 Views of another tensor's storage

We can get the second point in the tensor by providing the corresponding index:

```
# In[21]:
points = torch.tensor([[4.0, 1.0], [5.0, 3.0], [2.0, 1.0]])
second_point = points[1]
second_point.storage_offset()

# Out[21]:
2

# In[22]:
second_point.size()

# Out[22]:
torch.Size([2])
```

The resulting tensor has offset 2 in the storage (since we need to skip the first point, which has two items), and the size is an instance of the `Size` class containing one

element, since the tensor is one-dimensional. It's important to note that this is the same information contained in the `shape` property of tensor objects:

```
# In[23]:
second_point.shape

# Out[23]:
torch.Size([2])
```

The stride is a tuple indicating the number of elements in the storage that have to be skipped when the index is increased by 1 in each dimension. For instance, our `points` tensor has a stride of `(2, 1)`:

```
# In[24]:
points.stride()

# Out[24]:
(2, 1)
```

Accessing an element `i, j` in a 2D tensor results in accessing the `storage_offset + stride[0] * i + stride[1] * j` element in the storage. The offset will usually be zero; if this tensor is a view of a storage created to hold a larger tensor, the offset might be a positive value.

This indirection between `Tensor` and `Storage` makes some operations inexpensive, like transposing a tensor or extracting a subtensor, because they do not lead to memory reallocations. Instead, they consist of allocating a new `Tensor` object with a different value for size, storage offset, or stride.

We already extracted a subtensor when we indexed a specific point and saw the storage offset increasing. Let's see what happens to the size and stride as well:

```
# In[25]:
second_point = points[1]
second_point.size()

# Out[25]:
torch.Size([2])

# In[26]:
second_point.storage_offset()

# Out[26]:
2

# In[27]:
second_point.stride()

# Out[27]:
(1,)
```

The bottom line is that the subtensor has one less dimension, as we would expect, while still indexing the same storage as the original `points` tensor. This also means changing the subtensor will have a side effect on the original tensor:

```
# In[28]:
points = torch.tensor([[4.0, 1.0], [5.0, 3.0], [2.0, 1.0]])
second_point = points[1]
second_point[0] = 10.0
points

# Out[28]:
tensor([[ 4.,  1.],
        [10.,  3.],
        [ 2.,  1.]])
```

This might not always be desirable, so we can eventually clone the subtensor into a new tensor:

```
# In[29]:
points = torch.tensor([[4.0, 1.0], [5.0, 3.0], [2.0, 1.0]])
second_point = points[1].clone()
second_point[0] = 10.0
points

# Out[29]:
tensor([[4., 1.],
        [5., 3.],
        [2., 1.]])
```

3.8.2 Transposing without copying

Let's try transposing now. Let's take our `points` tensor, which has individual points in the rows and X and Y coordinates in the columns, and turn it around so that individual points are in the columns. We take this opportunity to introduce the `t` function, a shorthand alternative to `transpose` for two-dimensional tensors:

```
# In[30]:
points = torch.tensor([[4.0, 1.0], [5.0, 3.0], [2.0, 1.0]])
points

# Out[30]:
tensor([[4., 1.],
        [5., 3.],
        [2., 1.]])

# In[31]:
points_t = points.t()
points_t

# Out[31]:
tensor([[4., 5., 2.],
        [1., 3., 1.]])
```

TIP To help build a solid understanding of the mechanics of tensors, it may be a good idea to grab a pencil and a piece of paper and scribble diagrams like the one in figure 3.5 as we step through the code in this section.

We can easily verify that the two tensors share the same storage

```
# In[32]:
id(points.storage()) == id(points_t.storage())

# Out[32]:
True
```

and that they differ only in shape and stride:

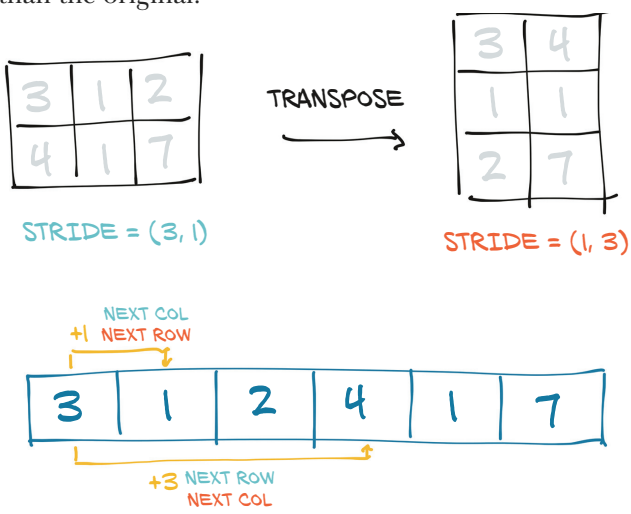
```
# In[33]:
points.stride()

# Out[33]:
(2, 1)
# In[34]:
points_t.stride()

# Out[34]:
(1, 2)
```

This tells us that increasing the first index by one in `points`—for example, going from `points[0,0]` to `points[1,0]`—will skip along the storage by two elements, while increasing the second index—from `points[0,0]` to `points[0,1]`—will skip along the storage by one. In other words, the storage holds the elements in the tensor sequentially row by row.

We can transpose `points` into `points_t`, as shown in figure 3.6. We change the order of the elements in the stride. After that, increasing the row (the first index of the tensor) will skip along the storage by one, just like when we were moving along columns in `points`. This is the very definition of transposing. No new memory is allocated: transposing is obtained only by creating a new `Tensor` instance with different stride ordering than the original.



gure 3.6 Transpose eration applied to a tensor

3.8.3 Transposing in higher dimensions

Transposing in PyTorch is not limited to matrices. We can transpose a multidimensional array by specifying the two dimensions along which transposing (flipping shape and stride) should occur:

```
# In[35]:
some_t = torch.ones(3, 4, 5)
transpose_t = some_t.transpose(0, 2)
some_t.shape

# Out[35]:
torch.Size([3, 4, 5])

# In[36]:
transpose_t.shape

# Out[36]:
torch.Size([5, 4, 3])

# In[37]:
some_t.stride()

# Out[37]:
(20, 5, 1)

# In[38]:
transpose_t.stride()

# Out[38]:
(1, 5, 20)
```

A tensor whose values are laid out in the storage starting from the rightmost dimension onward (that is, moving along rows for a 2D tensor) is defined as `contiguous`. Contiguous tensors are convenient because we can visit them efficiently in order without jumping around in the storage (improving data locality improves performance because of the way memory access works on modern CPUs). This advantage of course depends on the way algorithms visit.

3.8.4 Contiguous tensors

Some tensor operations in PyTorch only work on contiguous tensors, such as `view`, which we'll encounter in the next chapter. In that case, PyTorch will throw an informative exception and require us to call `contiguous` explicitly. It's worth noting that calling `contiguous` will do nothing (and will not hurt performance) if the tensor is already contiguous.

In our case, `points` is contiguous, while its transpose is not:

```
# In[39]:
points.is_contiguous()
```

```
# Out[39]:
True

# In[40]:
points_t.is_contiguous()

# Out[40]:
False
```

We can obtain a new contiguous tensor from a non-contiguous one using the `contiguous` method. The content of the tensor will be the same, but the stride will change, as will the storage:

```
# In[41]:
points = torch.tensor([[4.0, 1.0], [5.0, 3.0], [2.0, 1.0]])
points_t = points.t()
points_t

# Out[41]:
tensor([[4., 5., 2.],
        [1., 3., 1.]])

# In[42]:
points_t.storage()

# Out[42]:
 4.0
 1.0
 5.0
 3.0
 2.0
 1.0
[torch.FloatStorage of size 6]

# In[43]:
points_t.stride()

# Out[43]:
(1, 2)

# In[44]:
points_t_cont = points_t.contiguous()
points_t_cont

# Out[44]:
tensor([[4., 5., 2.],
        [1., 3., 1.]])

# In[45]:
points_t_cont.stride()

# Out[45]:
(3, 1)
```

```
# In[46]:
points_t_cont.storage()

# Out[46]:
 4.0
 5.0
 2.0
 1.0
 3.0
 1.0
[torch.FloatStorage of size 6]
```

Notice that the storage has been reshuffled in order for elements to be laid out row-by-row in the new storage. The stride has been changed to reflect the new layout.

As a refresher, figure 3.7 shows our diagram again. Hopefully it will all make sense now that we've taken a good look at how tensors are built.

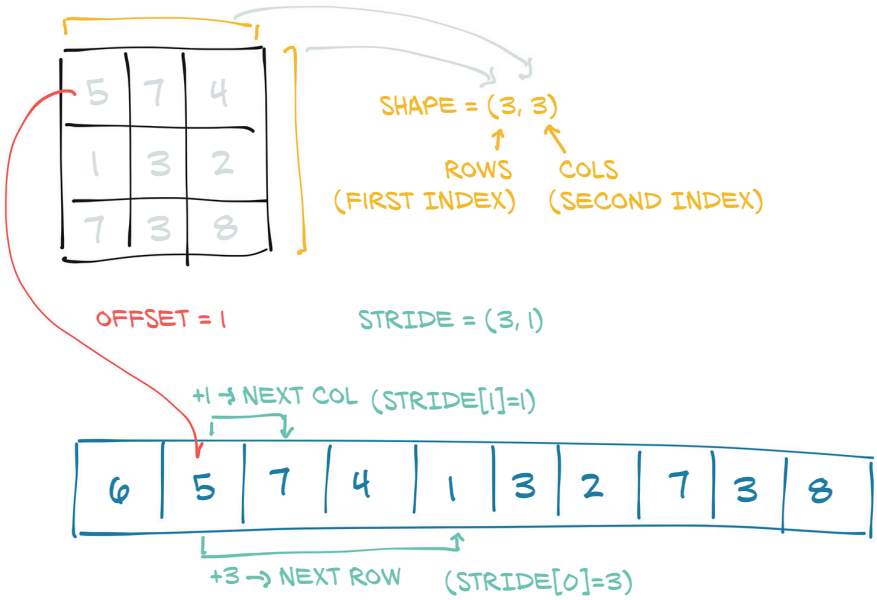


Figure 3.7 Relationship between a tensor's offset, size, and stride. Here the tensor is a view of a larger storage, like one that might have been allocated when creating a larger tensor.

3.9 Moving tensors to the GPU

So far in this chapter, when we've talked about storage, we've meant memory on the CPU. PyTorch tensors also can be stored on a different kind of processor: a graphics processing unit (GPU). Every PyTorch tensor can be transferred to (one of) the GPU(s) in order to perform massively parallel, fast computations. All operations that will be performed on the tensor will be carried out using GPU-specific routines that come with PyTorch.

PyTorch support for various GPUs

As of mid-2019, the main PyTorch releases only have acceleration on GPUs that have support for CUDA. PyTorch can run on AMD's ROCm (https://rocm.github.io), and the master repository provides support, but so far, you need to compile it yourself. (Before the regular build process, you need to run `tools/amd_build/build_amd.py` to translate the GPU code.) Support for Google's tensor processing units (TPUs) is a work in progress (https://github.com/pytorch/xla), with the current proof of concept available to the public in Google Colab: https://colab.research.google.com. Implementation of data structures and kernels on other GPU technologies, such as OpenCL, are not planned at the time of this writing.

3.9.1 Managing a tensor's device attribute

In addition to `dtype`, a PyTorch `Tensor` also has the notion of `device`, which is where on the computer the tensor data is placed. Here is how we can create a tensor on the GPU by specifying the corresponding argument to the constructor:

```
# In[64]:
points_gpu = torch.tensor([[4.0, 1.0], [5.0, 3.0], [2.0, 1.0]], device='cuda')
```

We could instead copy a tensor created on the CPU onto the GPU using the `to` method:

```
# In[65]:
points_gpu = points.to(device='cuda')
```

Doing so returns a new tensor that has the same numerical data, but stored in the RAM of the GPU, rather than in regular system RAM. Now that the data is stored locally on the GPU, we'll start to see the speedups mentioned earlier when performing mathematical operations on the tensor. In almost all cases, CPU- and GPU-based tensors expose the same user-facing API, making it much easier to write code that is agnostic to where, exactly, the heavy number crunching is running.

If our machine has more than one GPU, we can also decide on which GPU we allocate the tensor by passing a zero-based integer identifying the GPU on the machine, such as

```
# In[66]:
points_gpu = points.to(device='cuda:0')
```

At this point, any operation performed on the tensor, such as multiplying all elements by a constant, is carried out on the GPU:

```
# In[67]:
points = 2 * points
points_gpu = 2 * points.to(device='cuda')
```

Multiplication performed on the CPU

Multiplication performed on the GPU

Note that the `points_gpu` tensor is not brought back to the CPU once the result has been computed. Here's what happened in this line:

1. The `points` tensor is copied to the GPU.
2. A new tensor is allocated on the GPU and used to store the result of the multiplication.
3. A handle to that GPU tensor is returned.

Therefore, if we also add a constant to the result

```
# In[68]:
points_gpu = points_gpu + 4
```

the addition is still performed on the GPU, and no information flows to the CPU (unless we print or access the resulting tensor). In order to move the tensor back to the CPU, we need to provide a `cpu` argument to the `to` method, such as

```
# In[69]:
points_cpu = points_gpu.to(device='cpu')
```

We can also use the shorthand methods `cpu` and `cuda` instead of the `to` method to achieve the same goal:

```
# In[70]:
points_gpu = points.cuda()   <-- Defaults to GPU index 0
points_gpu = points.cuda(0)
points_cpu = points_gpu.cpu()
```

It's also worth mentioning that by using the `to` method, we can change the placement and the data type simultaneously by providing both `device` and `dtype` as arguments.

3.10 NumPy interoperability

We've mentioned NumPy here and there. While we do not consider NumPy a prerequisite for reading this book, we strongly encourage you to become familiar with NumPy due to its ubiquity in the Python data science ecosystem. PyTorch tensors can be converted to NumPy arrays and vice versa very efficiently. By doing so, we can take advantage of the huge swath of functionality in the wider Python ecosystem that has built up around the NumPy array type. This zero-copy interoperability with NumPy arrays is due to the storage system working with the Python buffer protocol (https://docs.python.org/3/c-api/buffer.html).

To get a NumPy array out of our `points` tensor, we just call

```
# In[55]:
points = torch.ones(3, 4)
points_np = points.numpy()
points_np

# Out[55]:
```

```
array([[1., 1., 1., 1.],
       [1., 1., 1., 1.],
       [1., 1., 1., 1.]], dtype=float32)
```

which will return a NumPy multidimensional array of the right size, shape, and numerical type. Interestingly, the returned array shares the same underlying buffer with the tensor storage. This means the `numpy` method can be effectively executed at basically no cost, as long as the data sits in CPU RAM. It also means modifying the NumPy array will lead to a change in the originating tensor. If the tensor is allocated on the GPU, PyTorch will make a copy of the content of the tensor into a NumPy array allocated on the CPU.

Conversely, we can obtain a PyTorch tensor from a NumPy array this way

```
# In[56]:
points = torch.from_numpy(points_np)
```

which will use the same buffer-sharing strategy we just described.

NOTE While the default numeric type in PyTorch is 32-bit floating-point, for NumPy it is 64-bit. As discussed in section 3.5.2, we usually want to use 32-bit floating-points, so we need to make sure we have tensors of `dtype` `torch.float` after converting.

3.11 Generalized tensors are tensors, too

For the purposes of this book, and for the vast majority of applications in general, tensors are multidimensional arrays, just as we've seen in this chapter. If we risk a peek under the hood of PyTorch, there is a twist: how the data is stored under the hood is separate from the tensor API we discussed in section 3.6. Any implementation that meets the contract of that API can be considered a tensor!

PyTorch will cause the right computation functions to be called regardless of whether our tensor is on the CPU or the GPU. This is accomplished through a *dispatching* mechanism, and that mechanism can cater to other tensor types by hooking up the user-facing API to the right backend functions. Sure enough, there are other kinds of tensors: some are specific to certain classes of hardware devices (like Google TPUs), and others have data-representation strategies that differ from the dense array style we've seen so far. For example, sparse tensors store only nonzero entries, along with index information. The PyTorch dispatcher on the left in figure 3.8 is designed to be extensible; the subsequent switching done to accommodate the various numeric types of figure 3.8 shown on the right is a fixed aspect of the implementation coded into each backend.

We will meet *quantized* tensors in chapter 15, which are implemented as another type of tensor with a specialized computational backend. Sometimes the usual tensors we use are called *dense* or *strided* to differentiate them from tensors using other memory layouts.

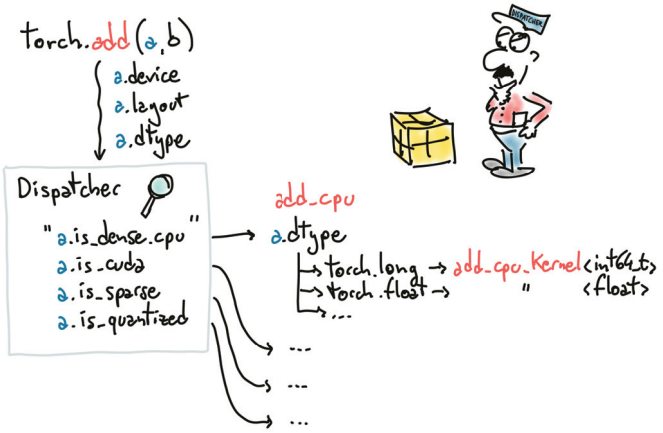


Figure 3.8 The dispatcher in PyTorch is one of its key infrastructure bits.

As with many things, the number of kinds of tensors has grown as PyTorch supports a broader range of hardware and applications. We can expect new kinds to continue to arise as people explore new ways to express and perform computations with PyTorch.

3.12 Serializing tensors

Creating a tensor on the fly is all well and good, but if the data inside is valuable, we will want to save it to a file and load it back at some point. After all, we don't want to have to retrain a model from scratch every time we start running our program! PyTorch uses `pickle` under the hood to serialize the tensor object, plus dedicated serialization code for the storage. Here's how we can save our `points` tensor to an ourpoints.t file:

```
# In[57]:
torch.save(points, '../data/p1ch3/ourpoints.t')
```

As an alternative, we can pass a file descriptor in lieu of the filename:

```
# In[58]:
with open('../data/p1ch3/ourpoints.t','wb') as f:
    torch.save(points, f)
```

Loading our points back is similarly a one-liner

```
# In[59]:
points = torch.load('../data/p1ch3/ourpoints.t')
```

or, equivalently,

```
# In[60]:
with open('../data/p1ch3/ourpoints.t','rb') as f:
    points = torch.load(f)
```

While we can quickly save tensors this way if we only want to load them with PyTorch, the file format itself is not interoperable: we can't read the tensor with software other than PyTorch. Depending on the use case, this may or may not be a limitation, but we should learn how to save tensors interoperably for those times when it is. We'll look next at how to do so.

3.12.1 Serializing to HDF5 with h5py

Every use case is unique, but we suspect needing to save tensors interoperably will be more common when introducing PyTorch into existing systems that already rely on different libraries. New projects probably won't need to do this as often.

For those cases when you need to, however, you can use the HDF5 format and library (www.hdfgroup.org/solutions/hdf5). HDF5 is a portable, widely supported format for representing serialized multidimensional arrays, organized in a nested key-value dictionary. Python supports HDF5 through the `h5py` library (www.h5py.org), which accepts and returns data in the form of NumPy arrays.

We can install `h5py` using

```
$ conda install h5py
```

At this point, we can save our `points` tensor by converting it to a NumPy array (at no cost, as we noted earlier) and passing it to the `create_dataset` function:

```
# In[61]:
import h5py

f = h5py.File('../data/p1ch3/ourpoints.hdf5', 'w')
dset = f.create_dataset('coords', data=points.numpy())
f.close()
```

Here `'coords'` is a key into the HDF5 file. We can have other keys—even nested ones. One of the interesting things in HDF5 is that we can index the dataset while on disk and access only the elements we're interested in. Let's suppose we want to load just the last two points in our dataset:

```
# In[62]:
f = h5py.File('../data/p1ch3/ourpoints.hdf5', 'r')
dset = f['coords']
last_points = dset[-2:]
```

The data is not loaded when the file is opened or the dataset is required. Rather, the data stays on disk until we request the second and last rows in the dataset. At that point, `h5py` accesses those two columns and returns a NumPy array-like object encapsulating that region in that dataset that behaves like a NumPy array and has the same API.

Owing to this fact, we can pass the returned object to the `torch.from_numpy` function to obtain a tensor directly. Note that in this case, the data is copied over to the tensor's storage:

```
# In[63]:
last_points = torch.from_numpy(dset[-2:])
f.close()
```

Once we're finished loading data, we close the file. Closing the HDFS file invalidates the datasets, and trying to access `dset` afterward will give an exception. As long as we stick to the order shown here, we are fine and can now work with the `last_points` tensor.

3.13 Conclusion

Now we have covered everything we need to get started with representing everything in floats. We'll cover other aspects of tensors—such as creating views of tensors; indexing tensors with other tensors; and broadcasting, which simplifies performing element-wise operations between tensors of different sizes or shapes—as needed along the way.

In chapter 4, we will learn how to represent real-world data in PyTorch. We will start with simple tabular data and move on to something more elaborate. In the process, we will get to know more about tensors.

3.14 Exercises

1. Create a tensor `a` from `list(range(9))`. Predict and then check the size, offset, and stride.
   a. Create a new tensor using `b = a.view(3, 3)`. What does `view` do? Check that `a` and `b` share the same storage.
   b. Create a tensor `c = b[1:,1:]`. Predict and then check the size, offset, and stride.
2. Pick a mathematical operation like cosine or square root. Can you find a corresponding function in the `torch` library?
   a. Apply the function element-wise to `a`. Why does it return an error?
   b. What operation is required to make the function work?
   c. Is there a version of your function that operates in place?

3.15 Summary

- Neural networks transform floating-point representations into other floating-point representations. The starting and ending representations are typically human interpretable, but the intermediate representations are less so.
- These floating-point representations are stored in tensors.
- Tensors are multidimensional arrays; they are the basic data structure in PyTorch.

- PyTorch has a comprehensive standard library for tensor creation, manipulation, and mathematical operations.
- Tensors can be serialized to disk and loaded back.
- All tensor operations in PyTorch can execute on the CPU as well as on the GPU, with no change in the code.
- PyTorch uses a trailing underscore to indicate that a function operates in place on a tensor (for example, `Tensor.sqrt_`).

4 Real-world data representation using tensors

This chapter covers

- Representing real-world data as PyTorch tensors
- Working with a range of data types
- Loading data from a file
- Converting data to tensors
- Shaping tensors so they can be used as inputs for neural network models

In the previous chapter, we learned that tensors are the building blocks for data in PyTorch. Neural networks take tensors as input and produce tensors as outputs. In fact, all operations within a neural network and during optimization are operations between tensors, and all parameters (for example, weights and biases) in a neural network are tensors. Having a good sense of how to perform operations on tensors and index them effectively is central to using tools like PyTorch successfully. Now

that you know the basics of tensors, your dexterity with them will grow as you make your way through the book.

Here's a question that we can already address: how do we take a piece of data, a video, or a line of text, and represent it with a tensor in a way that is appropriate for training a deep learning model? This is what we'll learn in this chapter. We'll cover different types of data with a focus on the types relevant to this book and show how to represent that data as tensors. Then we'll learn how to load the data from the most common on-disk formats and get a feel for those data types' structure so we can see how to prepare them for training a neural network. Often, our raw data won't be perfectly formed for the problem we'd like to solve, so we'll have a chance to practice our tensor-manipulation skills with a few more interesting tensor operations.

Each section in this chapter will describe a data type, and each will come with its own dataset. While we've structured the chapter so that each data type builds on the previous one, feel free to skip around a bit if you're so inclined.

We'll be using a lot of image and volumetric data through the rest of the book, since those are common data types and they reproduce well in book format. We'll also cover tabular data, time series, and text, as those will also be of interest to a number of our readers. Since a picture is worth a thousand words, we'll start with image data. We'll then demonstrate working with a three-dimensional array using medical data that represents patient anatomy as a volume. Next, we'll work with tabular data about wines, just like what we'd find in a spreadsheet. After that, we'll move to *ordered* tabular data, with a time-series dataset from a bike-sharing program. Finally, we'll dip our toes into text data from Jane Austen. Text data retains its ordered aspect but introduces the problem of representing words as arrays of numbers.

In every section, we will stop where a deep learning researcher would start: right before feeding the data to a model. We encourage you to keep these datasets; they will constitute excellent material for when we start learning how to train neural network models in the next chapter.

4.1 Working with images

The introduction of convolutional neural networks revolutionized computer vision (see http://mng.bz/zjMa), and image-based systems have since acquired a whole new set of capabilities. Problems that required complex pipelines of highly tuned algorithmic building blocks are now solvable at unprecedented levels of performance by training end-to-end networks using paired input-and-desired-output examples. In order to participate in this revolution, we need to be able to load an image from common image formats and then transform the data into a tensor representation that has the various parts of the image arranged in the way PyTorch expects.

An image is represented as a collection of scalars arranged in a regular grid with a height and a width (in pixels). We might have a single scalar per grid point (the pixel), which would be represented as a grayscale image; or multiple scalars per grid point, which would typically represent different colors, as we saw in the previous chapter, or different *features* like depth from a depth camera.

Scalars representing values at individual pixels are often encoded using 8-bit integers, as in consumer cameras. In medical, scientific, and industrial applications, it is not unusual to find higher numerical precision, such as 12-bit or 16-bit. This allows a wider range or increased sensitivity in cases where the pixel encodes information about a physical property, like bone density, temperature, or depth.

4.1.1 Adding color channels

We mentioned colors earlier. There are several ways to encode colors into numbers.[1] The most common is RGB, where a color is defined by three numbers representing the intensity of red, green, and blue. We can think of a color channel as a grayscale intensity map of only the color in question, similar to what you'd see if you looked at the scene in question using a pair of pure red sunglasses. Figure 4.1 shows a rainbow, where each of the RGB channels captures a certain portion of the spectrum (the figure is simplified, in that it elides things like the orange and yellow bands being represented as a combination of red and green).

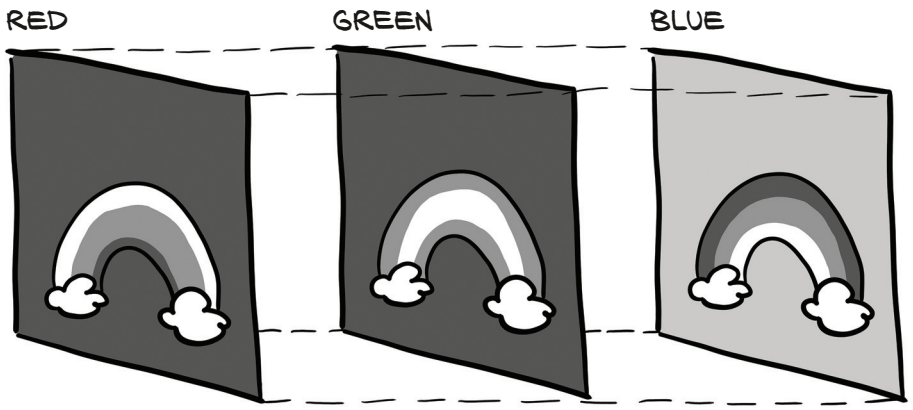


Figure 4.1 A rainbow, broken into red, green, and blue channels

The red band of the rainbow is brightest in the red channel of the image, while the blue channel has both the blue band of the rainbow and the sky as high-intensity. Note also that the white clouds are high-intensity in all three channels.

4.1.2 Loading an image file

Images come in several different file formats, but luckily there are plenty of ways to load images in Python. Let's start by loading a PNG image using the `imageio` module (code/p1ch4/1_image_dog.ipynb).

[1] This is something of an understatement: https://en.wikipedia.org/wiki/Color_model.

Listing 4.1 code/p1ch4/1_image_dog.ipynb

```
# In[2]:
import imageio

img_arr = imageio.imread('../data/p1ch4/image-dog/bobby.jpg')
img_arr.shape

# Out[2]:
(720, 1280, 3)
```

> **NOTE** We'll use `imageio` throughout the chapter because it handles different data types with a uniform API. For many purposes, using TorchVision is a great default choice to deal with image and video data. We go with `imageio` here for somewhat lighter exploration.

At this point, `img` is a NumPy array-like object with three dimensions: two spatial dimensions, width and height; and a third dimension corresponding to the red, green, and blue channels. Any library that outputs a NumPy array will suffice to obtain a PyTorch tensor. The only thing to watch out for is the layout of the dimensions. PyTorch modules dealing with image data require tensors to be laid out as $C \times H \times W$: channels, height, and width, respectively.

4.1.3 Changing the layout

We can use the tensor's `permute` method with the old dimensions for each new dimension to get to an appropriate layout. Given an input tensor $H \times W \times C$ as obtained previously, we get a proper layout by having channel 2 first and then channels 0 and 1:

```
# In[3]:
img = torch.from_numpy(img_arr)
out = img.permute(2, 0, 1)
```

We've seen this previously, but note that this operation does not make a copy of the tensor data. Instead, `out` uses the same underlying storage as `img` and only plays with the size and stride information at the tensor level. This is convenient because the operation is very cheap; but just as a heads-up: changing a pixel in `img` will lead to a change in `out`.

Note also that other deep learning frameworks use different layouts. For instance, originally TensorFlow kept the channel dimension last, resulting in an $H \times W \times C$ layout (it now supports multiple layouts). This strategy has pros and cons from a low-level performance standpoint, but for our concerns, it doesn't make a difference as long as we reshape our tensors properly.

So far, we have described a single image. Following the same strategy we've used for earlier data types, to create a dataset of multiple images to use as an input for our neural networks, we store the images in a batch along the first dimension to obtain an $N \times C \times H \times W$ tensor.

As a slightly more efficient alternative to using `stack` to build up the tensor, we can pre-allocate a tensor of appropriate size and fill it with images loaded from a directory, like so:

```
# In[4]:
batch_size = 3
batch = torch.zeros(batch_size, 3, 256, 256, dtype=torch.uint8)
```

This indicates that our batch will consist of three RGB images 256 pixels in height and 256 pixels in width. Notice the type of the tensor: we're expecting each color to be represented as an 8-bit integer, as in most photographic formats from standard consumer cameras. We can now load all PNG images from an input directory and store them in the tensor:

```
# In[5]:
import os

data_dir = '../data/p1ch4/image-cats/'
filenames = [name for name in os.listdir(data_dir)
             if os.path.splitext(name)[-1] == '.png']
for i, filename in enumerate(filenames):
    img_arr = imageio.imread(os.path.join(data_dir, filename))
    img_t = torch.from_numpy(img_arr)
    img_t = img_t.permute(2, 0, 1)
    img_t = img_t[:3]
    batch[i] = img_t
```

Here we keep only the first three channels. Sometimes images also have an alpha channel indicating transparency, but our network only wants RGB input.

4.1.4 Normalizing the data

We mentioned earlier that neural networks usually work with floating-point tensors as their input. Neural networks exhibit the best training performance when the input data ranges roughly from 0 to 1, or from -1 to 1 (this is an effect of how their building blocks are defined).

So a typical thing we'll want to do is cast a tensor to floating-point and normalize the values of the pixels. Casting to floating-point is easy, but normalization is trickier, as it depends on what range of the input we decide should lie between 0 and 1 (or -1 and 1). One possibility is to just divide the values of the pixels by 255 (the maximum representable number in 8-bit unsigned):

```
# In[6]:
batch = batch.float()
batch /= 255.0
```

Another possibility is to compute the mean and standard deviation of the input data and scale it so that the output has zero mean and unit standard deviation across each channel:

```
# In[7]:
n_channels = batch.shape[1]
for c in range(n_channels):
    mean = torch.mean(batch[:, c])
    std = torch.std(batch[:, c])
    batch[:, c] = (batch[:, c] - mean) / std
```

NOTE Here, we normalize just a single batch of images because we do not know yet how to operate on an entire dataset. In working with images, it is good practice to compute the mean and standard deviation on all the training data in advance and then subtract and divide by these fixed, precomputed quantities. We saw this in the preprocessing for the image classifier in section 2.1.4.

We can perform several other operations on inputs, such as geometric transformations like rotations, scaling, and cropping. These may help with training or may be required to make an arbitrary input conform to the input requirements of a network, like the size of the image. We will stumble on quite a few of these strategies in section 12.6. For now, just remember that you have image-manipulation options available.

4.2 3D images: Volumetric data

We've learned how to load and represent 2D images, like the ones we take with a camera. In some contexts, such as medical imaging applications involving, say, CT (computed tomography) scans, we typically deal with sequences of images stacked along the head-to-foot axis, each corresponding to a slice across the human body. In CT scans, the intensity represents the density of the different parts of the body—lungs, fat, water, muscle, and bone, in order of increasing density—mapped from dark to bright when the CT scan is displayed on a clinical workstation. The density at each point is computed from the amount of X-rays reaching a detector after crossing through the body, with some complex math to deconvolve the raw sensor data into the full volume.

CTs have only a single intensity channel, similar to a grayscale image. This means that often, the channel dimension is left out in native data formats; so, similar to the last section, the raw data typically has three dimensions. By stacking individual 2D slices into a 3D tensor, we can build volumetric data representing the 3D anatomy of a subject. Unlike what we saw in figure 4.1, the extra dimension in figure 4.2 represents an offset in physical space, rather than a particular band of the visible spectrum.

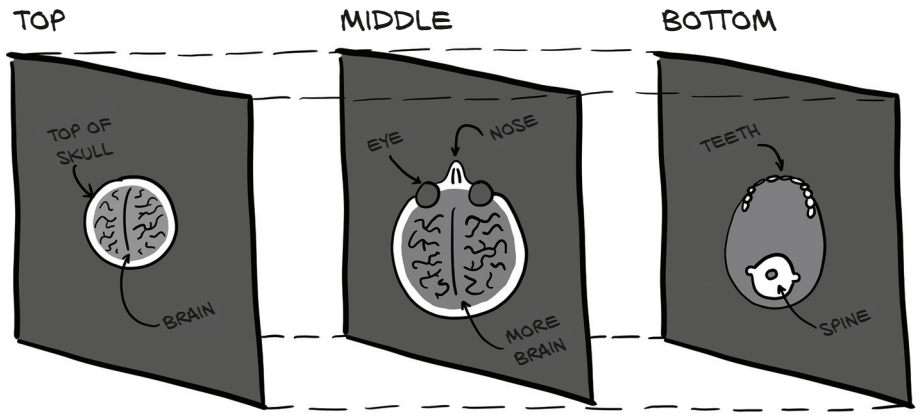


Figure 4.2 Slices of a CT scan, from the top of the head to the jawline

Part 2 of this book will be devoted to tackling a medical imaging problem in the real world, so we won't go into the details of medical-imaging data formats. For now, it suffices to say that there's no fundamental difference between a tensor storing volumetric data versus image data. We just have an extra dimension, *depth*, after the *channel* dimension, leading to a 5D tensor of shape $N \times C \times D \times H \times W$.

4.2.1 Loading a specialized format

Let's load a sample CT scan using the `volread` function in the `imageio` module, which takes a directory as an argument and assembles all Digital Imaging and Communications in Medicine (DICOM) files[2] in a series in a NumPy 3D array (code/p1ch4/2_volumetric_ct.ipynb).

Listing 4.2 code/p1ch4/2_volumetric_ct.ipynb

```
# In[2]:
import imageio

dir_path = "../data/p1ch4/volumetric-dicom/2-LUNG 3.0  B70f-04083"
vol_arr = imageio.volread(dir_path, 'DICOM')
vol_arr.shape

# Out[2]:
Reading DICOM (examining files): 1/99 files (1.0%99/99 files (100.0%)
  Found 1 correct series.
Reading DICOM (loading data): 31/99  (31.392/99  (92.999/99  (100.0%)

(99, 512, 512)
```

As was true in section 4.1.3, the layout is different from what PyTorch expects, due to having no channel information. So we'll have to make room for the `channel` dimension using `unsqueeze`:

```
# In[3]:
vol = torch.from_numpy(vol_arr).float()
vol = torch.unsqueeze(vol, 0)

vol.shape

# Out[3]:
torch.Size([1, 99, 512, 512])
```

At this point we could assemble a 5D dataset by stacking multiple volumes along the `batch` direction, just as we did in the previous section. We'll see a lot more CT data in part 2.

[2] From the Cancer Imaging Archive's CPTAC-LSCC collection: http://mng.bz/K21K.

4.3 Representing tabular data

The simplest form of data we'll encounter on a machine learning job is sitting in a spreadsheet, CSV file, or database. Whatever the medium, it's a table containing one row per sample (or record), where columns contain one piece of information about our sample.

At first we are going to assume there's no meaning to the order in which samples appear in the table: such a table is a collection of independent samples, unlike a time series, for instance, in which samples are related by a time dimension.

Columns may contain numerical values, like temperatures at specific locations; or labels, like a string expressing an attribute of the sample, like "blue." Therefore, tabular data is typically not homogeneous: different columns don't have the same type. We might have a column showing the weight of apples and another encoding their color in a label.

PyTorch tensors, on the other hand, are homogeneous. Information in PyTorch is typically encoded as a number, typically floating-point (though integer types and Boolean are supported as well). This numeric encoding is deliberate, since neural networks are mathematical entities that take real numbers as inputs and produce real numbers as output through successive application of matrix multiplications and nonlinear functions.

4.3.1 Using a real-world dataset

Our first job as deep learning practitioners is to encode heterogeneous, real-world data into a tensor of floating-point numbers, ready for consumption by a neural network. A large number of tabular datasets are freely available on the internet; see, for instance, https://github.com/caesar0301/awesome-public-datasets. Let's start with something fun: wine! The Wine Quality dataset is a freely available table containing chemical characterizations of samples of *vinho verde*, a wine from north Portugal, together with a sensory quality score. The dataset for white wines can be downloaded here: http://mng.bz/90Ol. For convenience, we also created a copy of the dataset on the Deep Learning with PyTorch Git repository, under data/p1ch4/tabular-wine.

The file contains a comma-separated collection of values organized in 12 columns preceded by a header line containing the column names. The first 11 columns contain values of chemical variables, and the last column contains the sensory quality score from 0 (very bad) to 10 (excellent). These are the column names in the order they appear in the dataset:

```
fixed acidity
volatile acidity
citric acid
residual sugar
chlorides
free sulfur dioxide
total sulfur dioxide
density
```

```
pH
sulphates
alcohol
quality
```

A possible machine learning task on this dataset is predicting the quality score from chemical characterization alone. Don't worry, though; machine learning is not going to kill wine tasting anytime soon. We have to get the training data from somewhere! As we can see in figure 4.3, we're hoping to find a relationship between one of the chemical columns in our data and the quality column. Here, we're expecting to see quality increase as sulfur decreases.

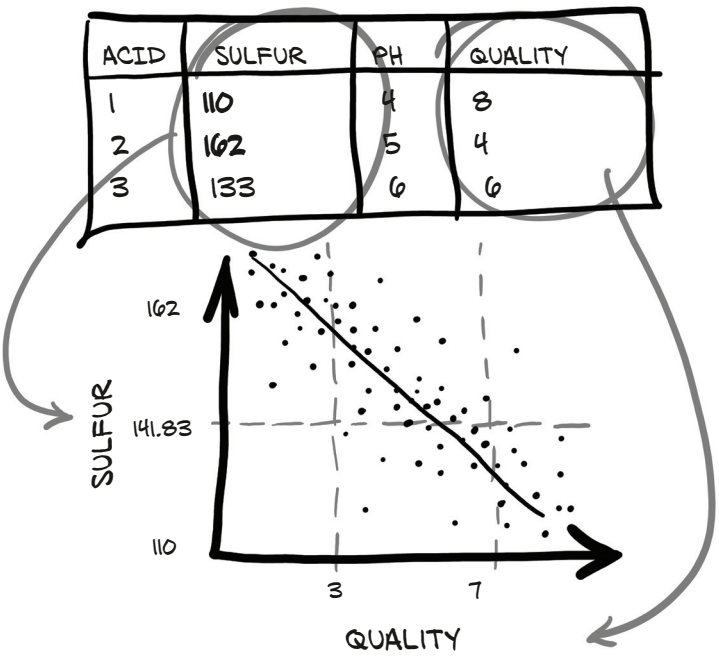


Figure 4.3 The (we hope) relationship between sulfur and quality in wine

4.3.2 Loading a wine data tensor

Before we can get to that, however, we need to be able to examine the data in a more usable way than opening the file in a text editor. Let's see how we can load the data using Python and then turn it into a PyTorch tensor. Python offers several options for quickly loading a CSV file. Three popular options are

- The `csv` module that ships with Python
- NumPy
- Pandas

The third option is the most time- and memory-efficient. However, we'll avoid introducing an additional library in our learning trajectory just because we need to load a file. Since we already introduced NumPy in the previous section, and PyTorch has excellent NumPy interoperability, we'll go with that. Let's load our file and turn the resulting NumPy array into a PyTorch tensor (code/p1ch4/3_tabular_wine.ipynb).

Listing 4.3 code/p1ch4/3_tabular_wine.ipynb

```
# In[2]:
import csv
wine_path = "../data/p1ch4/tabular-wine/winequality-white.csv"
wineq_numpy = np.loadtxt(wine_path, dtype=np.float32, delimiter=";",
                         skiprows=1)
wineq_numpy

# Out[2]:
array([[ 7.  ,  0.27,  0.36, ...,  0.45,  8.8 ,  6.  ],
       [ 6.3 ,  0.3 ,  0.34, ...,  0.49,  9.5 ,  6.  ],
       [ 8.1 ,  0.28,  0.4 , ...,  0.44, 10.1 ,  6.  ],
       ...,
       [ 6.5 ,  0.24,  0.19, ...,  0.46,  9.4 ,  6.  ],
       [ 5.5 ,  0.29,  0.3 , ...,  0.38, 12.8 ,  7.  ],
       [ 6.  ,  0.21,  0.38, ...,  0.32, 11.8 ,  6.  ]], dtype=float32)
```

Here we just prescribe what the type of the 2D array should be (32-bit floating-point), the delimiter used to separate values in each row, and the fact that the first line should not be read since it contains the column names. Let's check that all the data has been read

```
# In[3]:
col_list = next(csv.reader(open(wine_path), delimiter=';'))

wineq_numpy.shape, col_list

# Out[3]:
((4898, 12),
 ['fixed acidity',
  'volatile acidity',
  'citric acid',
  'residual sugar',
  'chlorides',
  'free sulfur dioxide',
  'total sulfur dioxide',
  'density',
  'pH',
  'sulphates',
  'alcohol',
  'quality'])
```

and proceed to convert the NumPy array to a PyTorch tensor:

```
# In[4]:
wineq = torch.from_numpy(wineq_numpy)

wineq.shape, wineq.dtype

# Out[4]:
(torch.Size([4898, 12]), torch.float32)
```

At this point, we have a floating-point `torch.Tensor` containing all the columns, including the last, which refers to the quality score.

Continuous, ordinal, and categorical values

We should be aware of three different kinds of numerical values as we attempt to make sense of our data.[3] The first kind is *continuous* values. These are the most intuitive when represented as numbers. They are strictly ordered, and a difference between various values has a strict meaning. Stating that package A is 2 kilograms heavier than package B, or that package B came from 100 miles farther away than A has a fixed meaning, regardless of whether package A is 3 kilograms or 10, or if B came from 200 miles away or 2,000. If you're counting or measuring something with units, it's probably a continuous value. The literature actually divides continuous values further: in the previous examples, it makes sense to say something is twice as heavy or three times farther away, so those values are said to be on a *ratio scale*. The time of day, on the other hand, does have the notion of difference, but it is not reasonable to claim that 6:00 is twice as late as 3:00; so time of day only offers an *interval scale*.

Next we have *ordinal* values. The strict ordering we have with continuous values remains, but the fixed relationship between values no longer applies. A good example of this is ordering a small, medium, or large drink, with small mapped to the value 1, medium 2, and large 3. The large drink is bigger than the medium, in the same way that 3 is bigger than 2, but it doesn't tell us anything about *how much* bigger. If we were to convert our 1, 2, and 3 to the actual volumes (say, 8, 12, and 24 fluid ounces), then they would switch to being interval values. It's important to remember that we can't "do math" on the values outside of ordering them; trying to average large = 3 and small = 1 does *not* result in a medium drink!

Finally, *categorical* values have neither ordering nor numerical meaning to their values. These are often just enumerations of possibilities assigned arbitrary numbers. Assigning water to 1, coffee to 2, soda to 3, and milk to 4 is a good example. There's no real logic to placing water first and milk last; they simply need distinct values to differentiate them. We could assign coffee to 10 and milk to –3, and there would be no significant change (though assigning values in the range $0..N-1$ will have advantages for one-hot encoding and the embeddings we'll discuss in section 4.5.4.) Because the numerical values bear no meaning, they are said to be on a *nominal scale*.

[3] As a starting point for a more in-depth discussion, refer to https://en.wikipedia.org/wiki/Level_of_measurement.

4.3.3 Representing scores

We could treat the score as a continuous variable, keep it as a real number, and perform a regression task, or treat it as a label and try to guess the label from the chemical analysis in a classification task. In both approaches, we will typically remove the score from the tensor of input data and keep it in a separate tensor, so that we can use the score as the ground truth without it being input to our model:

```
# In[5]:
data = wineq[:, :-1]
data, data.shape

# Out[5]:
(tensor([[ 7.00,  0.27,  ...,  0.45,  8.80],
         [ 6.30,  0.30,  ...,  0.49,  9.50],
         ...,
         [ 5.50,  0.29,  ...,  0.38, 12.80],
         [ 6.00,  0.21,  ...,  0.32, 11.80]]), torch.Size([4898, 11]))

# In[6]:
target = wineq[:, -1]
target, target.shape

# Out[6]:
(tensor([6., 6.,  ..., 7., 6.]), torch.Size([4898]))
```

Selects all rows and all columns except the last

Selects all rows and the last column

If we want to transform the `target` tensor in a tensor of labels, we have two options, depending on the strategy or what we use the categorical data for. One is simply to treat labels as an integer vector of scores:

```
# In[7]:
target = wineq[:, -1].long()
target

# Out[7]:
tensor([6, 6,  ..., 7, 6])
```

If targets were string labels, like *wine color*, assigning an integer number to each string would let us follow the same approach.

4.3.4 One-hot encoding

The other approach is to build a *one-hot encoding* of the scores: that is, encode each of the 10 scores in a vector of 10 elements, with all elements set to 0 but one, at a different index for each score. This way, a score of 1 could be mapped onto the vector `(1,0,0,0,0,0,0,0,0,0)`, a score of 5 onto `(0,0,0,0,1,0,0,0,0,0)`, and so on. Note that the fact that the score corresponds to the index of the nonzero element is purely incidental: we could shuffle the assignment, and nothing would change from a classification standpoint.

There's a marked difference between the two approaches. Keeping wine quality scores in an integer vector of scores induces an ordering on the scores—which might be totally appropriate in this case, since a score of 1 is lower than a score of 4. It also induces some sort of distance between scores: that is, the distance between 1 and 3 is the same as the distance between 2 and 4. If this holds for our quantity, then great. If, on the other hand, scores are purely discrete, like grape variety, one-hot encoding will be a much better fit, as there's no implied ordering or distance. One-hot encoding is also appropriate for quantitative scores when fractional values in between integer scores, like 2.4, make no sense for the application—for when the score is either *this* or *that*.

We can achieve one-hot encoding using the `scatter_` method, which fills the tensor with values from a source tensor along the indices provided as arguments:

```
# In[8]:
target_onehot = torch.zeros(target.shape[0], 10)

target_onehot.scatter_(1, target.unsqueeze(1), 1.0)

# Out[8]:
tensor([[0., 0.,  ..., 0., 0.],
        [0., 0.,  ..., 0., 0.],
        ...,
        [0., 0.,  ..., 0., 0.],
        [0., 0.,  ..., 0., 0.]])
```

Let's see what `scatter_` does. First, we notice that its name ends with an underscore. As you learned in the previous chapter, this is a convention in PyTorch that indicates the method will not return a new tensor, but will instead modify the tensor in place. The arguments for `scatter_` are as follows:

- The dimension along which the following two arguments are specified
- A column tensor indicating the indices of the elements to scatter
- A tensor containing the elements to scatter or a single scalar to scatter (1, in this case)

In other words, the previous invocation reads, "For each row, take the index of the target label (which coincides with the score in our case) and use it as the column index to set the value 1.0." The end result is a tensor encoding categorical information.

The second argument of `scatter_`, the index tensor, is required to have the same number of dimensions as the tensor we scatter into. Since `target_onehot` has two dimensions (4,898 × 10), we need to add an extra dummy dimension to `target` using `unsqueeze`:

```
# In[9]:
target_unsqueezed = target.unsqueeze(1)
target_unsqueezed

# Out[9]:
tensor([[6],
```

```
        [6],
        ...,
        [7],
        [6]])
```

The call to `unsqueeze` adds a *singleton* dimension, from a 1D tensor of 4,898 elements to a 2D tensor of size (4,898 × 1), without changing its contents—no extra elements are added; we just decided to use an extra index to access the elements. That is, we access the first element of `target` as `target[0]` and the first element of its unsqueezed counterpart as `target_unsqueezed[0,0]`.

PyTorch allows us to use class indices directly as targets while training neural networks. However, if we wanted to use the score as a categorical input to the network, we would have to transform it to a one-hot-encoded tensor.

4.3.5 When to categorize

Now we have seen ways to deal with both continuous and categorical data. You may wonder what the deal is with the ordinal case discussed in the earlier sidebar. There is no general recipe for it; most commonly, such data is either treated as categorical (losing the ordering part, and hoping that maybe our model will pick it up during training if we only have a few categories) or continuous (introducing an arbitrary notion of distance). We will do the latter for the weather situation in figure 4.5. We summarize our data mapping in a small flow chart in figure 4.4.

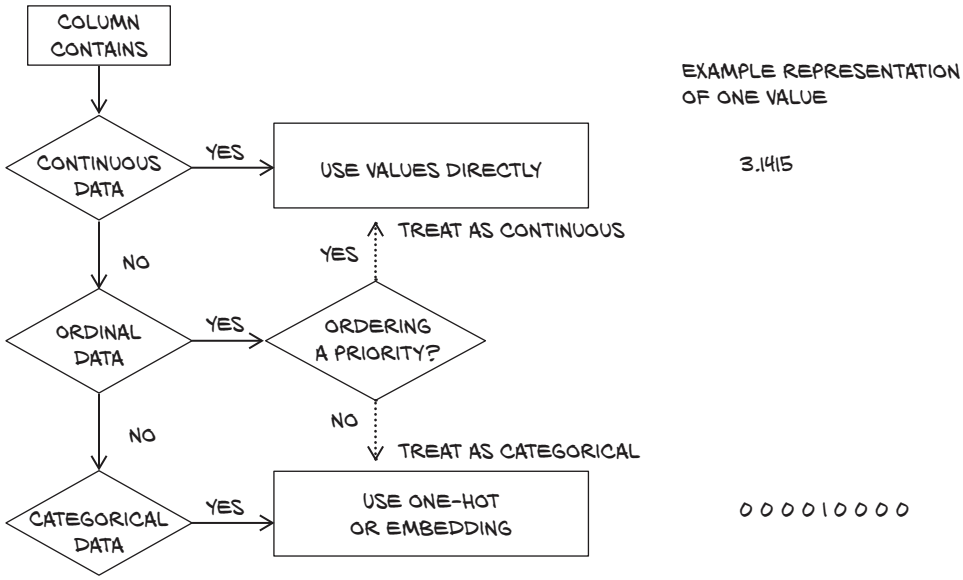


Figure 4.4 How to treat columns with continuous, ordinal, and categorical data

Let's go back to our `data` tensor, containing the 11 variables associated with the chemical analysis. We can use the functions in the PyTorch Tensor API to manipulate our data in tensor form. Let's first obtain the mean and standard deviations for each column:

```
# In[10]:
data_mean = torch.mean(data, dim=0)
data_mean

# Out[10]:
tensor([6.85e+00, 2.78e-01, 3.34e-01, 6.39e+00, 4.58e-02, 3.53e+01,
        1.38e+02, 9.94e-01, 3.19e+00, 4.90e-01, 1.05e+01])

# In[11]:
data_var = torch.var(data, dim=0)
data_var

# Out[11]:
tensor([7.12e-01, 1.02e-02, 1.46e-02, 2.57e+01, 4.77e-04, 2.89e+02,
        1.81e+03, 8.95e-06, 2.28e-02, 1.30e-02, 1.51e+00])
```

In this case, `dim=0` indicates that the reduction is performed along dimension 0. At this point, we can normalize the data by subtracting the mean and dividing by the standard deviation, which helps with the learning process (we'll discuss this in more detail in chapter 5, in section 5.4.4):

```
# In[12]:
data_normalized = (data - data_mean) / torch.sqrt(data_var)
data_normalized

# Out[12]:
tensor([[ 1.72e-01, -8.18e-02,  ..., -3.49e-01, -1.39e+00],
        [-6.57e-01,  2.16e-01,  ...,  1.35e-03, -8.24e-01],
        ...,
        [-1.61e+00,  1.17e-01,  ..., -9.63e-01,  1.86e+00],
        [-1.01e+00, -6.77e-01,  ..., -1.49e+00,  1.04e+00]])
```

4.3.6 Finding thresholds

Next, let's start to look at the data with an eye to seeing if there is an easy way to tell good and bad wines apart at a glance. First, we're going to determine which rows in `target` correspond to a score less than or equal to 3:

PyTorch also provides comparison functions, here torch.le(target, 3), but using operators seems to be a good standard.

```
# In[13]:
bad_indexes = target <= 3
bad_indexes.shape, bad_indexes.dtype, bad_indexes.sum()

# Out[13]:
(torch.Size([4898]), torch.bool, tensor(20))
```

Note that only 20 of the `bad_indexes` entries are set to `True`! By using a feature in PyTorch called *advanced indexing*, we can use a tensor with data type `torch.bool` to index the `data` tensor. This will essentially filter `data` to be only items (or rows) corresponding to `True` in the indexing tensor. The `bad_indexes` tensor has the same shape as `target`, with values of `False` or `True` depending on the outcome of the comparison between our threshold and each element in the original `target` tensor:

```
# In[14]:
bad_data = data[bad_indexes]
bad_data.shape

# Out[14]:
torch.Size([20, 11])
```

Note that the new `bad_data` tensor has 20 rows, the same as the number of rows with `True` in the `bad_indexes` tensor. It retains all 11 columns. Now we can start to get information about wines grouped into good, middling, and bad categories. Let's take the `.mean()` of each column:

```
# In[15]:
bad_data = data[target <= 3]
mid_data = data[(target > 3) & (target < 7)]
good_data = data[target >= 7]

bad_mean = torch.mean(bad_data, dim=0)
mid_mean = torch.mean(mid_data, dim=0)
good_mean = torch.mean(good_data, dim=0)

for i, args in enumerate(zip(col_list, bad_mean, mid_mean, good_mean)):
    print('{:2} {:20} {:6.2f} {:6.2f} {:6.2f}'.format(i, *args))

# Out[15]:
 0 fixed acidity          7.60   6.89   6.73
 1 volatile acidity       0.33   0.28   0.27
 2 citric acid            0.34   0.34   0.33
 3 residual sugar         6.39   6.71   5.26
 4 chlorides              0.05   0.05   0.04
 5 free sulfur dioxide   53.33  35.42  34.55
 6 total sulfur dioxide 170.60 141.83 125.25
 7 density                0.99   0.99   0.99
 8 pH                     3.19   3.18   3.22
 9 sulphates              0.47   0.49   0.50
10 alcohol               10.34  10.26  11.42
```

For Boolean NumPy arrays and PyTorch tensors, the & operator does a logical "and" operation.

It looks like we're on to something here: at first glance, the bad wines seem to have higher total sulfur dioxide, among other differences. We could use a threshold on total sulfur dioxide as a crude criterion for discriminating good wines from bad ones. Let's get the indexes where the total sulfur dioxide column is below the midpoint we calculated earlier, like so:

```
# In[16]:
total_sulfur_threshold = 141.83
total_sulfur_data = data[:,6]
predicted_indexes = torch.lt(total_sulfur_data, total_sulfur_threshold)

predicted_indexes.shape, predicted_indexes.dtype, predicted_indexes.sum()

# Out[16]:
(torch.Size([4898]), torch.bool, tensor(2727))
```

This means our threshold implies that just over half of all the wines are going to be high quality. Next, we'll need to get the indexes of the actually good wines:

```
# In[17]:
actual_indexes = target > 5

actual_indexes.shape, actual_indexes.dtype, actual_indexes.sum()

# Out[17]:
(torch.Size([4898]), torch.bool, tensor(3258))
```

Since there are about 500 more actually good wines than our threshold predicted, we already have hard evidence that it's not perfect. Now we need to see how well our predictions line up with the actual rankings. We will perform a logical "and" between our prediction indexes and the actual good indexes (remember that each is just an array of zeros and ones) and use that intersection of wines-in-agreement to determine how well we did:

```
# In[18]:
n_matches = torch.sum(actual_indexes & predicted_indexes).item()
n_predicted = torch.sum(predicted_indexes).item()
n_actual = torch.sum(actual_indexes).item()

n_matches, n_matches / n_predicted, n_matches / n_actual

# Out[18]:
(2018, 0.74000733406674, 0.6193984039287906)
```

We got around 2,000 wines right! Since we predicted 2,700 wines, this gives us a 74% chance that if we predict a wine to be high quality, it actually is. Unfortunately, there are 3,200 good wines, and we only identified 61% of them. Well, we got what we signed up for; that's barely better than random! Of course, this is all very naive: we know for sure that multiple variables contribute to wine quality, and the relationships between the values of these variables and the outcome (which could be the actual score, rather than a binarized version of it) is likely more complicated than a simple threshold on a single value.

Indeed, a simple neural network would overcome all of these limitations, as would a lot of other basic machine learning methods. We'll have the tools to tackle this problem after the next two chapters, once we have learned how to build our first neural

network from scratch. We will also revisit how to better grade our results in chapter 12. Let's move on to other data types for now.

4.4 Working with time series

In the previous section, we covered how to represent data organized in a flat table. As we noted, every row in the table was independent from the others; their order did not matter. Or, equivalently, there was no column that encoded information about what rows came earlier and what came later.

Going back to the wine dataset, we could have had a "year" column that allowed us to look at how wine quality evolved year after year. Unfortunately, we don't have such data at hand, but we're working hard on manually collecting the data samples, bottle by bottle. (Stuff for our second edition.) In the meantime, we'll switch to another interesting dataset: data from a Washington, D.C., bike-sharing system reporting the hourly count of rental bikes in 2011–2012 in the Capital Bikeshare system, along with weather and seasonal information (available here: http://mng.bz/jgOx). Our goal will be to take a flat, 2D dataset and transform it into a 3D one, as shown in figure 4.5.

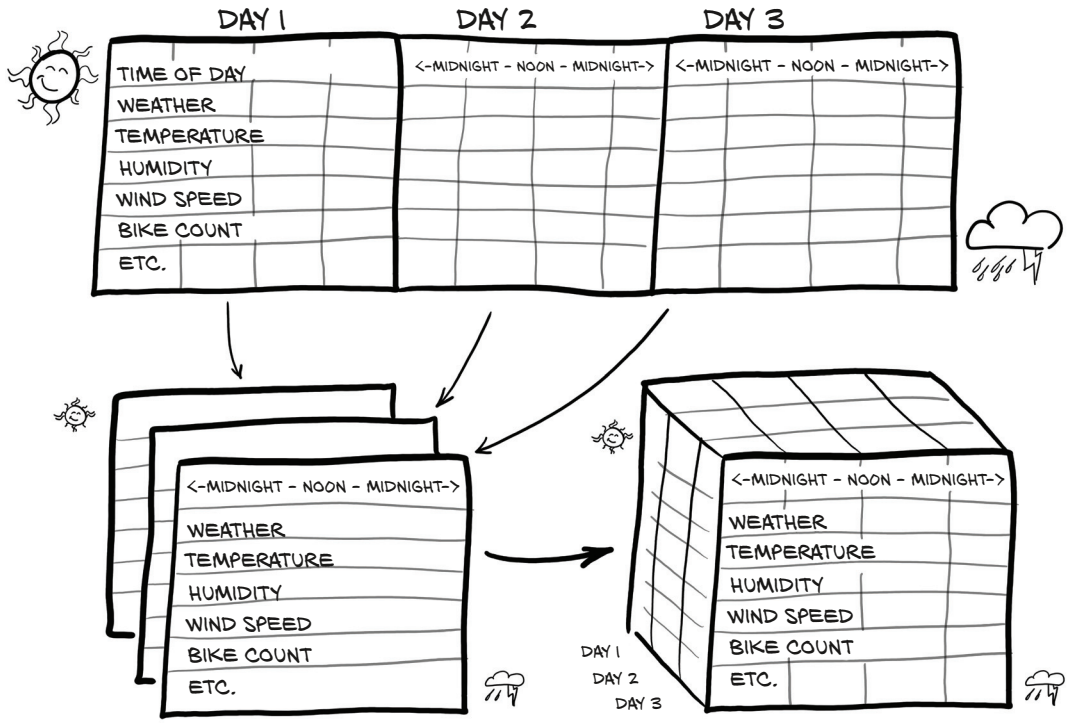


Figure 4.5 Transforming a 1D, multichannel dataset into a 2D, multichannel dataset by separating the date and hour of each sample into separate axes

4.4.1 Adding a time dimension

In the source data, each row is a separate hour of data (figure 4.5 shows a transposed version of this to better fit on the printed page). We want to change the row-per-hour organization so that we have one axis that increases at a rate of one day per index increment, and another axis that represents the hour of the day (independent of the date). The third axis will be our different columns of data (weather, temperature, and so on).

Let's load the data (code/p1ch4/4_time_series_bikes.ipynb).

Listing 4.4 code/p1ch4/4_time_series_bikes.ipynb

```
# In[2]:
bikes_numpy = np.loadtxt(
    "../data/p1ch4/bike-sharing-dataset/hour-fixed.csv",
    dtype=np.float32,
    delimiter=",",
    skiprows=1,
    converters={1: lambda x: float(x[8:10])})
bikes = torch.from_numpy(bikes_numpy)
bikes
```

Converts date strings to numbers corresponding to the day of the month in column 1

```
# Out[2]:
tensor([[1.0000e+00, 1.0000e+00,  ..., 1.3000e+01, 1.6000e+01],
        [2.0000e+00, 1.0000e+00,  ..., 3.2000e+01, 4.0000e+01],
        ...,
        [1.7378e+04, 3.1000e+01,  ..., 4.8000e+01, 6.1000e+01],
        [1.7379e+04, 3.1000e+01,  ..., 3.7000e+01, 4.9000e+01]])
```

For every hour, the dataset reports the following variables:

- Index of record: `instant`
- Day of month: `day`
- Season: `season` (`1`: spring, `2`: summer, `3`: fall, `4`: winter)
- Year: `yr` (`0`: 2011, `1`: 2012)
- Month: `mnth` (`1` to `12`)
- Hour: `hr` (`0` to `23`)
- Holiday status: `holiday`
- Day of the week: `weekday`
- Working day status: `workingday`
- Weather situation: `weathersit` (`1`: clear, `2`:mist, `3`: light rain/snow, `4`: heavy rain/snow)
- Temperature in °C: `temp`
- Perceived temperature in °C: `atemp`
- Humidity: `hum`
- Wind speed: `windspeed`
- Number of casual users: `casual`
- Number of registered users: `registered`
- Count of rental bikes: `cnt`

In a time series dataset such as this one, rows represent successive time-points: there is a dimension along which they are ordered. Sure, we could treat each row as independent and try to predict the number of circulating bikes based on, say, a particular time of day regardless of what happened earlier. However, the existence of an ordering gives us the opportunity to exploit causal relationships across time. For instance, it allows us to predict bike rides at one time based on the fact that it was raining at an earlier time. For the time being, we're going to focus on learning how to turn our bike-sharing dataset into something that our neural network will be able to ingest in fixed-size chunks.

This neural network model will need to see a number of sequences of values for each different quantity, such as ride count, time of day, temperature, and weather conditions: N parallel sequences of size C. C stands for *channel*, in neural network parlance, and is the same as *column* for 1D data like we have here. The N dimension represents the time axis, here one entry per hour.

4.4.2 Shaping the data by time period

We might want to break up the two-year dataset into wider observation periods, like days. This way we'll have N (for *number of samples*) collections of C sequences of length L. In other words, our time series dataset would be a tensor of dimension 3 and shape $N \times C \times L$. The C would remain our 17 channels, while L would be 24: 1 per hour of the day. There's no particular reason why we *must* use chunks of 24 hours, though the general daily rhythm is likely to give us patterns we can exploit for predictions. We could also use $7 \times 24 = 168$ hour blocks to chunk by week instead, if we desired. All of this depends, naturally, on our dataset having the right size—the number of rows must be a multiple of 24 or 168. Also, for this to make sense, we cannot have gaps in the time series.

Let's go back to our bike-sharing dataset. The first column is the index (the global ordering of the data), the second is the date, and the sixth is the time of day. We have everything we need to create a dataset of daily sequences of ride counts and other exogenous variables. Our dataset is already sorted, but if it were not, we could use `torch.sort` on it to order it appropriately.

> **NOTE** The version of the file we're using, hour-fixed.csv, has had some processing done to include rows missing from the original dataset. We presume that the missing hours had zero bike active (they were typically in the early morning hours).

All we have to do to obtain our daily hours dataset is view the same tensor in batches of 24 hours. Let's take a look at the shape and strides of our `bikes` tensor:

```
# In[3]:
bikes.shape, bikes.stride()

# Out[3]:
(torch.Size([17520, 17]), (17, 1))
```

That's 17,520 hours, 17 columns. Now let's reshape the data to have 3 axes—day, hour, and then our 17 columns:

```
# In[4]:
daily_bikes = bikes.view(-1, 24, bikes.shape[1])
daily_bikes.shape, daily_bikes.stride()

# Out[4]:
(torch.Size([730, 24, 17]), (408, 17, 1))
```

What happened here? First, `bikes.shape[1]` is 17, the number of columns in the `bikes` tensor. But the real crux of this code is the call to `view`, which is really important: it changes the way the tensor looks at the same data as contained in storage.

As you learned in the previous chapter, calling `view` on a tensor returns a new tensor that changes the number of dimensions and the striding information, without changing the storage. This means we can rearrange our tensor at basically zero cost, because no data will be copied. Our call to `view` requires us to provide the new shape for the returned tensor. We use `-1` as a placeholder for "however many indexes are left, given the other dimensions and the original number of elements."

Remember also from the previous chapter that storage is a contiguous, linear container for numbers (floating-point, in this case). Our `bikes` tensor will have each row stored one after the other in its corresponding storage. This is confirmed by the output from the call to `bikes.stride()` earlier.

For `daily_bikes`, the stride is telling us that advancing by 1 along the hour dimension (the second dimension) requires us to advance by 17 places in the storage (or one set of columns); whereas advancing along the day dimension (the first dimension) requires us to advance by a number of elements equal to the length of a row in the storage times 24 (here, 408, which is 17×24).

We see that the rightmost dimension is the number of columns in the original dataset. Then, in the middle dimension, we have time, split into chunks of 24 sequential hours. In other words, we now have N sequences of L hours in a day, for C channels. To get to our desired $N \times C \times L$ ordering, we need to transpose the tensor:

```
# In[5]:
daily_bikes = daily_bikes.transpose(1, 2)
daily_bikes.shape, daily_bikes.stride()

# Out[5]:
(torch.Size([730, 17, 24]), (408, 1, 17))
```

Now let's apply some of the techniques we learned earlier to this dataset.

4.4.3 Ready for training

The "weather situation" variable is ordinal. It has four levels: `1` for good weather, and `4` for, er, really bad. We could treat this variable as categorical, with levels interpreted as labels, or as a continuous variable. If we decided to go with categorical, we would turn

the variable into a one-hot-encoded vector and concatenate the columns with the dataset.[4]

In order to make it easier to render our data, we're going to limit ourselves to the first day for a moment. We initialize a zero-filled matrix with a number of rows equal to the number of hours in the day and number of columns equal to the number of weather levels:

```
# In[6]:
first_day = bikes[:24].long()
weather_onehot = torch.zeros(first_day.shape[0], 4)
first_day[:,9]

# Out[6]:
tensor([1, 1, 1, 1, 1, 2, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 3, 3, 2, 2,
        2, 2])
```

Then we scatter ones into our matrix according to the corresponding level at each row. Remember the use of `unsqueeze` to add a singleton dimension as we did in the previous sections:

```
# In[7]:
weather_onehot.scatter_(
    dim=1,
    index=first_day[:,9].unsqueeze(1).long() - 1,
    value=1.0)

# Out[7]:
tensor([[1., 0., 0., 0.],
        [1., 0., 0., 0.],
        ...,
        [0., 1., 0., 0.],
        [0., 1., 0., 0.]])
```

Decreases the values by 1 because weather situation ranges from 1 to 4, while indices are 0-based

Our day started with weather "1" and ended with "2," so that seems right.

Last, we concatenate our matrix to our original dataset using the `cat` function. Let's look at the first of our results:

```
# In[8]:
torch.cat((bikes[:24], weather_onehot), 1)[:1]

# Out[8]:
tensor([[ 1.0000,  1.0000,  1.0000,  0.0000,  1.0000,  0.0000,  0.0000,
          6.0000,  0.0000,  1.0000,  0.2400,  0.2879,  0.8100,  0.0000,
          3.0000, 13.0000, 16.0000,  1.0000,  0.0000,  0.0000,  0.0000]])
```

[4] This could also be a case where it is useful to go beyond the main path. Speculatively, we could also try to reflect *like categorical, but with order* more directly by generalizing one-hot encodings to mapping the ith of our four categories here to a vector that has ones in the positions $0 \ldots i$ and zeros beyond that. Or—similar to the embeddings we discussed in section 4.5.4—we could take partial sums of embeddings, in which case it might make sense to make those positive. As with many things we encounter in practical work, this could be a place where *trying what works for others* and then experimenting in a systematic fashion is a good idea.

Here we prescribed our original `bikes` dataset and our one-hot-encoded "weather situation" matrix to be concatenated along the *column* dimension (that is, 1). In other words, the columns of the two datasets are stacked together; or, equivalently, the new one-hot-encoded columns are appended to the original dataset. For `cat` to succeed, it is required that the tensors have the same size along the other dimensions—the *row* dimension, in this case. Note that our new last four columns are `1, 0, 0, 0`, exactly as we would expect with a weather value of 1.

We could have done the same with the reshaped `daily_bikes` tensor. Remember that it is shaped (*B*, *C*, *L*), where *L* = 24. We first create the zero tensor, with the same *B* and *L*, but with the number of additional columns as *C*:

```
# In[9]:
daily_weather_onehot = torch.zeros(daily_bikes.shape[0], 4,
                                   daily_bikes.shape[2])
daily_weather_onehot.shape

# Out[9]:
torch.Size([730, 4, 24])
```

Then we scatter the one-hot encoding into the tensor in the *C* dimension. Since this operation is performed in place, only the content of the tensor will change:

```
# In[10]:
daily_weather_onehot.scatter_(
    1, daily_bikes[:,9,:].long().unsqueeze(1) - 1, 1.0)
daily_weather_onehot.shape

# Out[10]:
torch.Size([730, 4, 24])
```

And we concatenate along the *C* dimension:

```
# In[11]:
daily_bikes = torch.cat((daily_bikes, daily_weather_onehot), dim=1)
```

We mentioned earlier that this is not the only way to treat our "weather situation" variable. Indeed, its labels have an ordinal relationship, so we could pretend they are special values of a continuous variable. We could just transform the variable so that it runs from 0.0 to 1.0:

```
# In[12]:
daily_bikes[:, 9, :] = (daily_bikes[:, 9, :] - 1.0) / 3.0
```

As we mentioned in the previous section, rescaling variables to the [0.0, 1.0] interval or the [-1.0, 1.0] interval is something we'll want to do for all quantitative variables, like `temperature` (column 10 in our dataset). We'll see why later; for now, let's just say that this is beneficial to the training process.

There are multiple possibilities for rescaling variables. We can either map their range to [0.0, 1.0]

```
# In[13]:
temp = daily_bikes[:, 10, :]
temp_min = torch.min(temp)
temp_max = torch.max(temp)
daily_bikes[:, 10, :] = ((daily_bikes[:, 10, :] - temp_min)
                         / (temp_max - temp_min))
```

or subtract the mean and divide by the standard deviation:

```
# In[14]:
temp = daily_bikes[:, 10, :]
daily_bikes[:, 10, :] = ((daily_bikes[:, 10, :] - torch.mean(temp))
                         / torch.std(temp))
```

In the latter case, our variable will have 0 mean and unitary standard deviation. If our variable were drawn from a Gaussian distribution, 68% of the samples would sit in the [-1.0, 1.0] interval.

Great: we've built another nice dataset, and we've seen how to deal with time series data. For this tour d'horizon, it's important only that we got an idea of how a time series is laid out and how we can wrangle the data in a form that a network will digest.

Other kinds of data look like a time series, in that there is a strict ordering. Top two on the list? Text and audio. We'll take a look at text next, and the "Conclusion" section has links to additional examples for audio.

4.5 Representing text

Deep learning has taken the field of natural language processing (NLP) by storm, particularly using models that repeatedly consume a combination of new input and previous model output. These models are called *recurrent neural networks* (RNNs), and they have been applied with great success to text categorization, text generation, and automated translation systems. More recently, a class of networks called *transformers* with a more flexible way to incorporate past information has made a big splash. Previous NLP workloads were characterized by sophisticated multistage pipelines that included rules encoding the grammar of a language.[5] Now, state-of-the-art work trains networks end to end on large corpora starting from scratch, letting those rules emerge from the data. For the last several years, the most-used automated translation systems available as services on the internet have been based on deep learning.

Our goal in this section is to turn text into something a neural network can process: a tensor of numbers, just like our previous cases. If we can do that and later choose the right architecture for our text-processing job, we'll be in the position of doing NLP with PyTorch. We see right away how powerful this all is: we can achieve

[5] Nadkarni et al., "Natural language processing: an introduction," JAMIA, http://mng.bz/8pJP. See also https://en.wikipedia.org/wiki/Natural-language_processing.

state-of-the-art performance on a number of tasks in different domains *with the same PyTorch tools*; we just need to cast our problem in the right form. The first part of this job is reshaping the data.

4.5.1 Converting text to numbers

There are two particularly intuitive levels at which networks operate on text: at the character level, by processing one character at a time, and at the word level, where individual words are the finest-grained entities to be seen by the network. The technique with which we encode text information into tensor form is the same whether we operate at the character level or the word level. And it's not magic, either. We stumbled upon it earlier: one-hot encoding.

Let's start with a character-level example. First, let's get some text to process. An amazing resource here is Project Gutenberg (www.gutenberg.org), a volunteer effort to digitize and archive cultural work and make it available for free in open formats, including plain text files. If we're aiming at larger-scale corpora, the Wikipedia corpus stands out: it's the complete collection of Wikipedia articles, containing 1.9 billion words and more than 4.4 million articles. Several other corpora can be found at the English Corpora website (www.english-corpora.org).

Let's load Jane Austen's *Pride and Prejudice* from the Project Gutenberg website: www.gutenberg.org/files/1342/1342-0.txt. We'll just save the file and read it in (code/p1ch4/5_text_jane_austen.ipynb).

Listing 4.5 code/p1ch4/5_text_jane_austen.ipynb

```
# In[2]:
with open('../data/p1ch4/jane-austen/1342-0.txt', encoding='utf8') as f:
    text = f.read()
```

4.5.2 One-hot-encoding characters

There's one more detail we need to take care of before we proceed: encoding. This is a pretty vast subject, and we will just touch on it. Every written character is represented by a code: a sequence of bits of appropriate length so that each character can be uniquely identified. The simplest such encoding is ASCII (American Standard Code for Information Interchange), which dates back to the 1960s. ASCII encodes 128 characters using 128 integers. For instance, the letter *a* corresponds to binary 1100001 or decimal 97, the letter *b* to binary 1100010 or decimal 98, and so on. The encoding fits 8 bits, which was a big bonus in 1965.

> **NOTE** 128 characters are clearly not enough to account for all the glyphs, accents, ligatures, and so on that are needed to properly represent written text in languages other than English. To this end, a number of encodings have been developed that use a larger number of bits as code for a wider range of characters. That wider range of characters was standardized as Unicode, which maps all known characters to numbers, with the representation

in bits of those numbers provided by a specific encoding. Popular encodings are UTF-8, UTF-16, and UTF-32, in which the numbers are a sequence of 8-, 16-, or 32-bit integers, respectively. Strings in Python 3.x are Unicode strings.

We are going to one-hot encode our characters. It is instrumental to limit the one-hot encoding to a character set that is useful for the text being analyzed. In our case, since we loaded text in English, it is safe to use ASCII and deal with a small encoding. We could also make all of the characters lowercase, to reduce the number of different characters in our encoding. Similarly, we could screen out punctuation, numbers, or other characters that aren't relevant to our expected kinds of text. This may or may not make a practical difference to a neural network, depending on the task at hand.

At this point, we need to parse through the characters in the text and provide a one-hot encoding for each of them. Each character will be represented by a vector of length equal to the number of different characters in the encoding. This vector will contain all zeros except a one at the index corresponding to the location of the character in the encoding.

We first split our text into a list of lines and pick an arbitrary line to focus on:

```
# In[3]:
lines = text.split('\n')
line = lines[200]
line

# Out[3]:
'"Impossible, Mr. Bennet, impossible, when I am not acquainted with him'
```

Let's create a tensor that can hold the total number of one-hot-encoded characters for the whole line:

```
# In[4]:
letter_t = torch.zeros(len(line), 128)
letter_t.shape

# Out[4]:
torch.Size([70, 128])
```

128 hardcoded due to the limits of ASCII

Note that `letter_t` holds a one-hot-encoded character per row. Now we just have to set a one on each row in the correct position so that each row represents the correct character. The index where the one has to be set corresponds to the index of the character in the encoding:

```
# In[5]:
for i, letter in enumerate(line.lower().strip()):
    letter_index = ord(letter) if ord(letter) < 128 else 0
    letter_t[i][letter_index] = 1
```

The text uses directional double quotes, which are not valid ASCII, so we screen them out here.

4.5.3 One-hot encoding whole words

We have one-hot encoded our sentence into a representation that a neural network could digest. Word-level encoding can be done the same way by establishing a vocabulary and one-hot encoding sentences—sequences of words—along the rows of our tensor. Since a vocabulary has many words, this will produce very wide encoded vectors, which may not be practical. We will see in the next section that there is a more efficient way to represent text at the word level, using *embeddings*. For now, let's stick with one-hot encodings and see what happens.

We'll define `clean_words`, which takes text and returns it in lowercase and stripped of punctuation. When we call it on our "Impossible, Mr. Bennet" `line`, we get the following:

```
# In[6]:
def clean_words(input_str):
    punctuation = '.,;:"!?”“_-'
    word_list = input_str.lower().replace('\n',' ').split()
    word_list = [word.strip(punctuation) for word in word_list]
    return word_list

words_in_line = clean_words(line)
line, words_in_line

# Out[6]:
('“Impossible, Mr. Bennet, impossible, when I am not acquainted with him',
 ['impossible',
  'mr',
  'bennet',
  'impossible',
  'when',
  'i',
  'am',
  'not',
  'acquainted',
  'with',
  'him'])
```

Next, let's build a mapping of words to indexes in our encoding:

```
# In[7]:
word_list = sorted(set(clean_words(text)))
word2index_dict = {word: i for (i, word) in enumerate(word_list)}

len(word2index_dict), word2index_dict['impossible']

# Out[7]:
(7261, 3394)
```

Note that `word2index_dict` is now a dictionary with words as keys and an integer as a value. We will use it to efficiently find the index of a word as we one-hot encode it. Let's now focus on our sentence: we break it up into words and one-hot encode it—

that is, we populate a tensor with one one-hot-encoded vector per word. We create an empty vector and assign the one-hot-encoded values of the word in the sentence:

```
# In[8]:
word_t = torch.zeros(len(words_in_line), len(word2index_dict))
for i, word in enumerate(words_in_line):
    word_index = word2index_dict[word]
    word_t[i][word_index] = 1
    print('{:2} {:4} {}'.format(i, word_index, word))

print(word_t.shape)


# Out[8]:
 0 3394 impossible
 1 4305 mr
 2  813 bennet
 3 3394 impossible
 4 7078 when
 5 3315 i
 6  415 am
 7 4436 not
 8  239 acquainted
 9 7148 with
10 3215 him
torch.Size([11, 7261])
```

At this point, `tensor` represents one sentence of length 11 in an encoding space of size 7,261, the number of words in our dictionary. Figure 4.6 compares the gist of our two options for splitting text (and using the embeddings we'll look at in the next section).

The choice between character-level and word-level encoding leaves us to make a trade-off. In many languages, there are significantly fewer characters than words: representing characters has us representing just a few classes, while representing words requires us to represent a very large number of classes and, in any practical application, deal with words that are not in the dictionary. On the other hand, words convey much more meaning than individual characters, so a representation of words is considerably more informative by itself. Given the stark contrast between these two options, it is perhaps unsurprising that intermediate ways have been sought, found, and applied with great success: for example, the *byte pair encoding* method[6] starts with a dictionary of individual letters but then iteratively adds the most frequently observed pairs to the dictionary until it reaches a prescribed dictionary size. Our example sentence might then be split into tokens like this:[7]

```
?Im|pos|s|ible|,|?Mr|.|?B|en|net|,|?impossible|,|?when|?I|?am|?not|➥
?acquainted|?with|?him
```

[6] Most commonly implemented by the subword-nmt and SentencePiece libraries. The conceptual drawback is that the representation of a sequence of characters is no longer unique.

[7] This is from a SentencePiece tokenizer trained on a machine translation dataset.

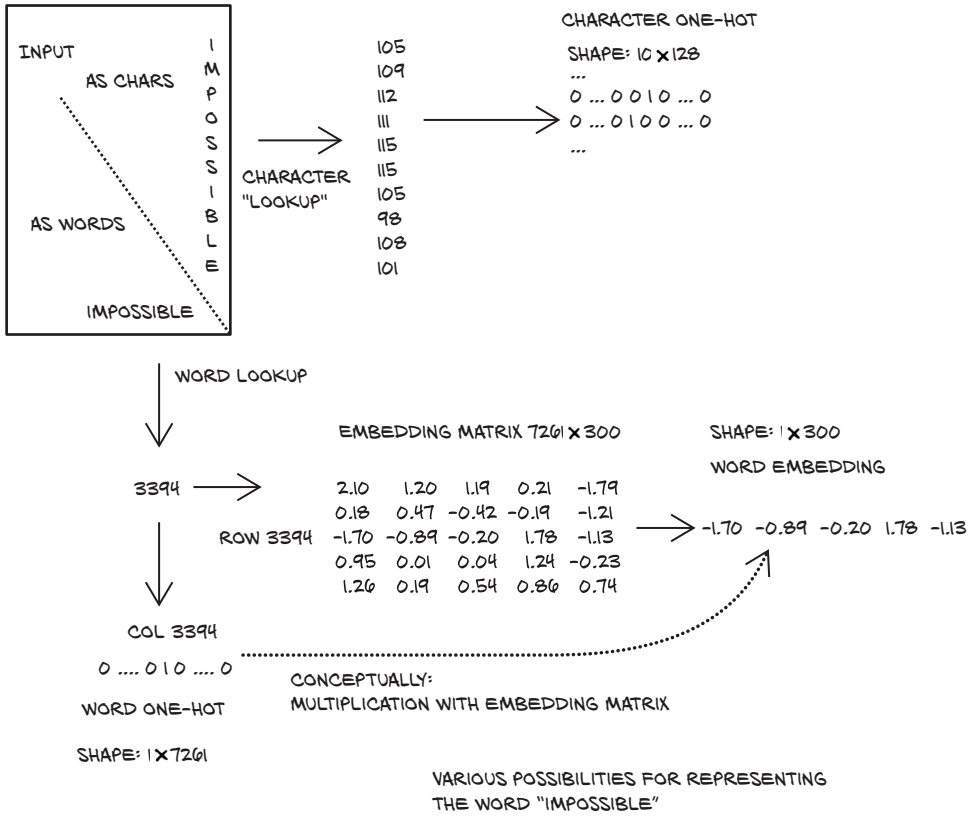


Figure 4.6 Three ways to encode a word

For most things, our mapping is just splitting by words. But the rarer parts—the capitalized *Impossible* and the name *Bennet*—are composed of subunits.

4.5.4 Text embeddings

One-hot encoding is a very useful technique for representing categorical data in tensors. However, as we have anticipated, one-hot encoding starts to break down when the number of items to encode is effectively unbound, as with words in a corpus. In just one book, we had over 7,000 items!

We certainly could do some work to deduplicate words, condense alternate spellings, collapse past and future tenses into a single token, and that kind of thing. Still, a general-purpose English-language encoding would be *huge*. Even worse, every time we encountered a new word, we would have to add a new column to the vector, which would mean adding a new set of weights to the model to account for that new vocabulary entry—which would be painful from a training perspective.

How can we compress our encoding down to a more manageable size and put a cap on the size growth? Well, instead of vectors of many zeros and a single one, we can

use vectors of floating-point numbers. A vector of, say, 100 floating-point numbers can indeed represent a large number of words. The trick is to find an effective way to map individual words into this 100-dimensional space in a way that facilitates downstream learning. This is called an *embedding*.

In principle, we could simply iterate over our vocabulary and generate a set of 100 random floating-point numbers for each word. This would work, in that we could cram a very large vocabulary into just 100 numbers, but it would forgo any concept of distance between words based on meaning or context. A model using this word embedding would have to deal with very little structure in its input vectors. An ideal solution would be to generate the embedding in such a way that words used in similar contexts mapped to nearby regions of the embedding.

Well, if we were to design a solution to this problem by hand, we might decide to build our embedding space by choosing to map basic nouns and adjectives along the axes. We can generate a 2D space where axes map to nouns—*fruit* (0.0-0.33), *flower* (0.33-0.66), and *dog* (0.66-1.0)—and adjectives—*red* (0.0-0.2), *orange* (0.2-0.4), *yellow* (0.4-0.6), *white* (0.6-0.8), and *brown* (0.8-1.0). Our goal is to take actual fruit, flowers, and dogs and lay them out in the embedding.

As we start embedding words, we can map *apple* to a number in the *fruit* and *red* quadrant. Likewise, we can easily map *tangerine*, *lemon*, *lychee*, and *kiwi* (to round out our list of colorful fruits). Then we can start on flowers, and assign *rose*, *poppy*, *daffodil*, *lily*, and … Hmm. Not many brown flowers out there. Well, *sunflower* can get *flower*, *yellow*, and *brown*, and then *daisy* can get *flower*, *white*, and *yellow*. Perhaps we should update *kiwi* to map close to *fruit*, *brown*, and *green*.[8] For dogs and color, we can embed *redbone* near *red*; uh, *fox* perhaps for *orange*; *golden retriever* for *yellow*, *poodle* for *white*, and … most kinds of dogs are *brown*.

Now our embeddings look like figure 4.7. While doing this manually isn't really feasible for a large corpus, note that although we had an embedding size of 2, we described 15 different words *besides the base 8* and could probably cram in quite a few more if we took the time to be creative about it.

As you've probably already guessed, this kind of work can be automated. By processing a large corpus of organic text, embeddings similar to the one we just discussed can be generated. The main differences are that there are 100 to 1,000 elements in the embedding vector and that axes do not map directly to concepts: rather, conceptually similar words map in neighboring regions of an embedding space whose axes are arbitrary floating-point dimensions.

While the exact algorithms[9] used are a bit out of scope for what we're wanting to focus on here, we'd just like to mention that embeddings are often generated using neural networks, trying to predict a word from nearby words (the context) in a sentence. In this case, we could start from one-hot-encoded words and use a (usually

[8] Actually, with our 1D view of color, this is not possible, as *sunflower*'s *yellow* and *brown* will average to *white*—but you get the idea, and it does work better in higher dimensions.

[9] One example is word2vec: https://code.google.com/archive/p/word2vec.

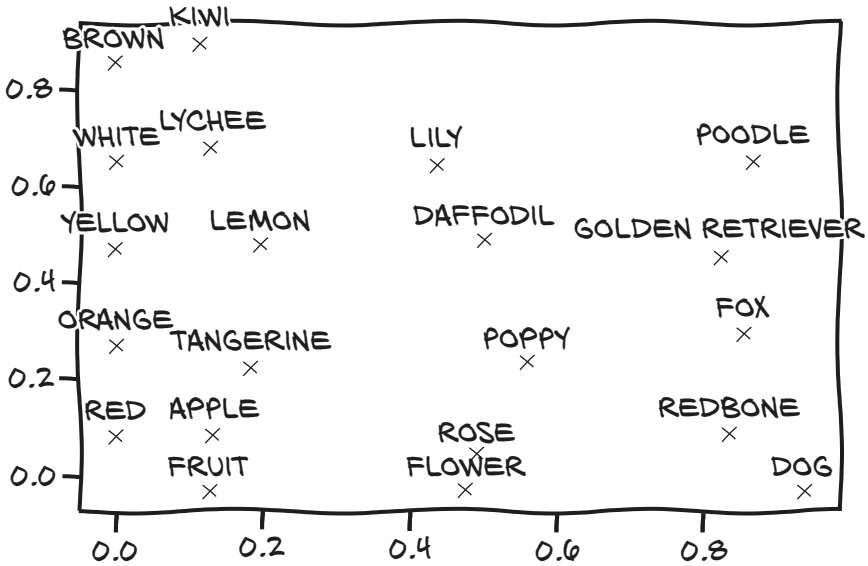


Figure 4.7 Our manual word embeddings

rather shallow) neural network to generate the embedding. Once the embedding was available, we could use it for downstream tasks.

One interesting aspect of the resulting embeddings is that similar words end up not only clustered together, but also having consistent spatial relationships with other words. For example, if we were to take the embedding vector for *apple* and begin to add and subtract the vectors for other words, we could begin to perform analogies like *apple - red - sweet + yellow + sour* and end up with a vector very similar to the one for *lemon*.

More contemporary embedding models—with BERT and GPT-2 making headlines even in mainstream media—are much more elaborate and are context sensitive: that is, the mapping of a word in the vocabulary to a vector is not fixed but depends on the surrounding sentence. Yet they are often used just like the simpler *classic* embeddings we've touched on here.

4.5.5 Text embeddings as a blueprint

Embeddings are an essential tool for when a large number of entries in the vocabulary have to be represented by numeric vectors. But we won't be using text and text embeddings in this book, so you might wonder why we introduce them here. We believe that how text is represented and processed can also be seen as an example for dealing with categorical data in general. Embeddings are useful wherever one-hot encoding becomes cumbersome. Indeed, in the form described previously, they are an efficient way of representing one-hot encoding immediately followed by multiplication with the matrix containing the embedding vectors as rows.

In non-text applications, we usually do not have the ability to construct the embeddings beforehand, but we will start with the random numbers we eschewed earlier and consider improving them part of our learning problem. This is a standard technique—so much so that embeddings are a prominent alternative to one-hot encodings for any categorical data. On the flip side, even when we deal with text, improving the prelearned embeddings while solving the problem at hand has become a common practice.[10]

When we are interested in co-occurrences of observations, the word embeddings we saw earlier can serve as a blueprint, too. For example, recommender systems—customers who liked our book also bought …—use the items the customer already interacted with as the context for predicting what else will spark interest. Similarly, processing text is perhaps the most common, well-explored task dealing with sequences; so, for example, when working on tasks with time series, we might look for inspiration in what is done in natural language processing.

4.6 Conclusion

We've covered a lot of ground in this chapter. We learned to load the most common types of data and shape them for consumption by a neural network. Of course, there are more data formats in the wild than we could hope to describe in a single volume. Some, like medical histories, are too complex to cover here. Others, like audio and video, were deemed less crucial for the path of this book. If you're interested, however, we provide short examples of audio and video tensor creation in bonus Jupyter Notebooks provided on the book's website (www.manning.com/books/deep-learning-with-pytorch) and in our code repository (https://github.com/deep-learning-with-pytorch/dlwpt-code/tree/master/p1ch4).

Now that we're familiar with tensors and how to store data in them, we can move on to the next step towards the goal of the book: teaching you to train deep neural networks! The next chapter covers the mechanics of learning for simple linear models.

4.7 Exercises

1. Take several pictures of red, blue, and green items with your phone or other digital camera (or download some from the internet, if a camera isn't available).
   a. Load each image, and convert it to a tensor.
   b. For each image tensor, use the `.mean()` method to get a sense of how bright the image is.
   c. Take the mean of each channel of your images. Can you identify the red, green, and blue items from only the channel averages?

[10] This goes by the name *fine-tuning*.

2. Select a relatively large file containing Python source code.
   a. Build an index of all the words in the source file (feel free to make your tokenization as simple or as complex as you like; we suggest starting with replacing `r"[^a-zA-Z0-9_]+"` with spaces).
   b. Compare your index with the one we made for *Pride and Prejudice*. Which is larger?
   c. Create the one-hot encoding for the source code file.
   d. What information is lost with this encoding? How does that information compare to what's lost in the *Pride and Prejudice* encoding?

4.8 Summary

- Neural networks require data to be represented as multidimensional numerical tensors, often 32-bit floating-point.
- In general, PyTorch expects data to be laid out along specific dimensions according to the model architecture—for example, convolutional versus recurrent. We can reshape data effectively with the PyTorch tensor API.
- Thanks to how the PyTorch libraries interact with the Python standard library and surrounding ecosystem, loading the most common types of data and converting them to PyTorch tensors is convenient.
- Images can have one or many channels. The most common are the red-green-blue channels of typical digital photos.
- Many images have a per-channel bit depth of 8, though 12 and 16 bits per channel are not uncommon. These bit depths can all be stored in a 32-bit floating-point number without loss of precision.
- Single-channel data formats sometimes omit an explicit channel dimension.
- Volumetric data is similar to 2D image data, with the exception of adding a third dimension (depth).
- Converting spreadsheets to tensors can be very straightforward. Categorical- and ordinal-valued columns should be handled differently from interval-valued columns.
- Text or categorical data can be encoded to a one-hot representation through the use of dictionaries. Very often, embeddings give good, efficient representations.

5 The mechanics of learning

This chapter covers

- Understanding how algorithms can learn from data
- Reframing learning as parameter estimation, using differentiation and gradient descent
- Walking through a simple learning algorithm
- How PyTorch supports learning with autograd

With the blooming of machine learning that has occurred over the last decade, the notion of machines that learn from experience has become a mainstream theme in both technical and journalistic circles. Now, how is it exactly that a machine learns? What are the mechanics of this process—or, in words, what is the *algorithm* behind it? From the point of view of an observer, a learning algorithm is presented with input data that is paired with desired outputs. Once learning has occurred, that algorithm will be capable of producing correct outputs when it is fed new data that is *similar enough* to the input data it was trained on. With deep learning, this process works even when the input data and the desired output are *far* from each other: when they come from different domains, like an image and a sentence describing it, as we saw in chapter 2.

5.1 A timeless lesson in modeling

Building models that allow us to explain input/output relationships dates back centuries at least. When Johannes Kepler, a German mathematical astronomer (1571–1630), figured out his three laws of planetary motion in the early 1600s, he based them on data collected by his mentor Tycho Brahe during naked-eye observations (yep, seen with the naked eye and written on a piece of paper). Not having Newton's law of gravitation at his disposal (actually, Newton used Kepler's work to figure things out), Kepler extrapolated the simplest possible geometric model that could fit the data. And, by the way, it took him six years of staring at data that didn't make sense to him, together with incremental realizations, to finally formulate these laws.[1] We can see this process in figure 5.1.

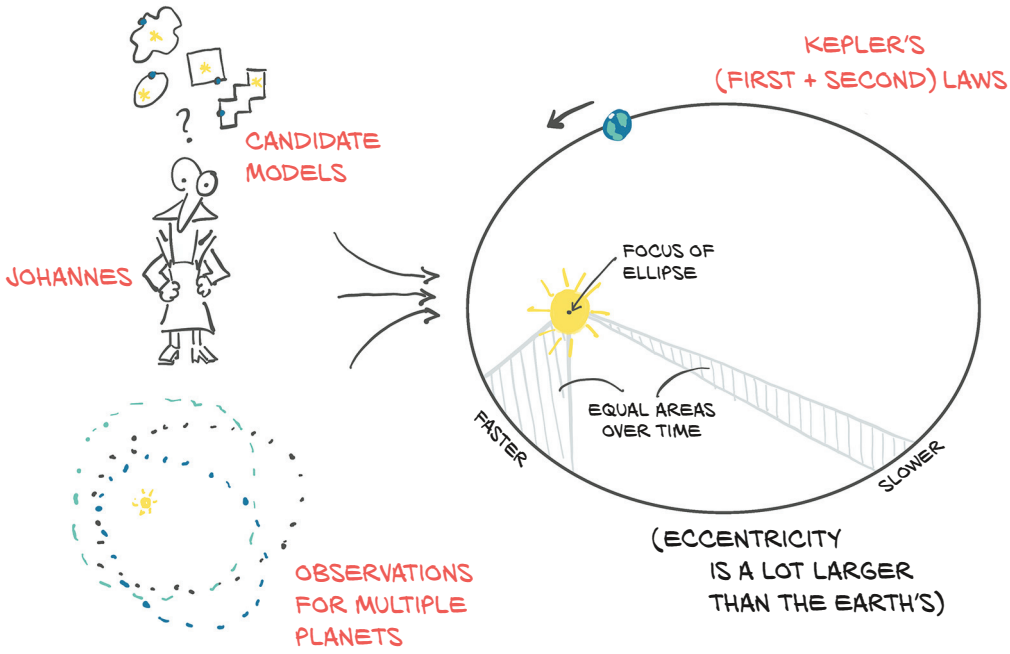


Figure 5.1 Johannes Kepler considers multiple candidate models that might fit the data at hand, settling on an ellipse.

Kepler's first law reads: "The orbit of every planet is an ellipse with the Sun at one of the two *foci*." He didn't know what caused orbits to be ellipses, but given a set of observations for a planet (or a moon of a large planet, like Jupiter), he could estimate the shape (the *eccentricity*) and size (the *semi-latus rectum*) of the ellipse. With those two parameters computed from the data, he could tell where the planet might be during

[1] As recounted by physicist Michael Fowler: http://mng.bz/K2Ej.

its journey in the sky. Once he figured out the second law—"A line joining a planet and the Sun sweeps out equal areas during equal intervals of time"—he could also tell *when* a planet would be at a particular point in space, given observations in time.[2]

So, how did Kepler estimate the eccentricity and size of the ellipse without computers, pocket calculators, or even calculus, none of which had been invented yet? We can learn how from Kepler's own recollection, in his book *New Astronomy*, or from how J. V. Field put it in his series of articles, "The origins of proof," (http://mng.bz/9007):

> *Essentially, Kepler had to try different shapes, using a certain number of observations to find the curve, then use the curve to find some more positions, for times when he had observations available, and then check whether these calculated positions agreed with the observed ones.*
>
> —J. V. Field

So let's sum things up. Over six years, Kepler

1. Got lots of good data from his friend Brahe (not without some struggle)
2. Tried to visualize the heck out of it, because he felt there was something fishy going on
3. Chose the simplest possible model that had a chance to fit the data (an ellipse)
4. Split the data so that he could work on part of it and keep an independent set for validation
5. Started with a tentative eccentricity and size for the ellipse and iterated until the model fit the observations
6. Validated his model on the independent observations
7. Looked back in disbelief

There's a data science handbook for you, all the way from 1609. The history of science is literally constructed on these seven steps. And we have learned over the centuries that deviating from them is a recipe for disaster.[3]

This is exactly what we will set out to do in order to *learn* something from data. In fact, in this book there is virtually no difference between saying that we'll *fit* the data or that we'll make an algorithm *learn* from data. The process always involves a function with a number of unknown parameters whose values are estimated from data: in short, a *model*.

We can argue that *learning from data* presumes the underlying model is not engineered to solve a specific problem (as was the ellipse in Kepler's work) and is instead capable of approximating a much wider family of functions. A neural network would have predicted Tycho Brahe's trajectories really well without requiring Kepler's flash of insight to try fitting the data to an ellipse. However, Sir Isaac Newton would have had a much harder time deriving his laws of gravitation from a generic model.

---

[2] Understanding the details of Kepler's laws is not needed to understand this chapter, but you can find more information at https://en.wikipedia.org/wiki/Kepler%27s_laws_of_planetary_motion.

[3] Unless you're a theoretical physicist ;).

In this book, we're interested in models that are not engineered for solving a specific narrow task, but that can be automatically adapted to specialize themselves for any one of many similar tasks using input and output pairs—in other words, general models trained on data relevant to the specific task at hand. In particular, PyTorch is designed to make it easy to create models for which the derivatives of the fitting error, with respect to the parameters, can be expressed analytically. No worries if this last sentence didn't make any sense at all; coming next, we have a full section that hopefully clears it up for you.

This chapter is about how to automate generic function-fitting. After all, this is what we do with deep learning—deep neural networks being the generic functions we're talking about—and PyTorch makes this process as simple and transparent as possible. In order to make sure we get the key concepts right, we'll start with a model that is a lot simpler than a deep neural network. This will allow us to understand the mechanics of learning algorithms from first principles in this chapter, so we can move to more complicated models in chapter 6.

5.2 Learning is just parameter estimation

In this section, we'll learn how we can take data, choose a model, and estimate the parameters of the model so that it will give good predictions on new data. To do so, we'll leave the intricacies of planetary motion and divert our attention to the second-hardest problem in physics: calibrating instruments.

Figure 5.2 shows the high-level overview of what we'll implement by the end of the chapter. Given input data and the corresponding desired outputs (ground truth), as well as initial values for the weights, the model is fed input data (forward pass), and a measure of the error is evaluated by comparing the resulting outputs to the ground truth. In order to optimize the parameter of the model—its *weights*—the change in the error following a unit change in weights (that is, the *gradient* of the error with respect to the parameters) is computed using the chain rule for the derivative of a composite function (backward pass). The value of the weights is then updated in the direction that leads to a decrease in the error. The procedure is repeated until the error, evaluated on unseen data, falls below an acceptable level. If what we just said sounds obscure, we've got a whole chapter to clear things up. By the time we're done, all the pieces will fall into place, and this paragraph will make perfect sense.

We're now going to take a problem with a noisy dataset, build a model, and implement a learning algorithm for it. When we start, we'll be doing everything by hand, but by the end of the chapter we'll be letting PyTorch do all the heavy lifting for us. When we finish the chapter, we will have covered many of the essential concepts that underlie training deep neural networks, even if our motivating example is very simple and our model isn't actually a neural network (yet!).

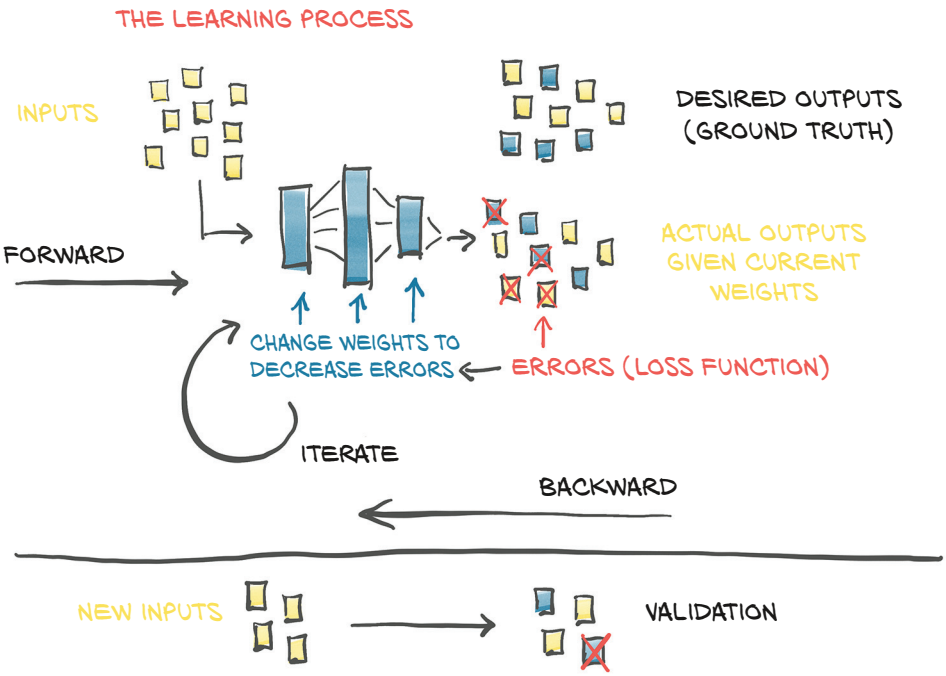


Figure 5.2 Our mental model of the learning process

5.2.1 A hot problem

We just got back from a trip to some obscure location, and we brought back a fancy, wall-mounted analog thermometer. It looks great, and it's a perfect fit for our living room. Its only flaw is that it doesn't show units. Not to worry, we've got a plan: we'll build a dataset of readings and corresponding temperature values in our favorite units, choose a model, adjust its weights iteratively until a measure of the error is low enough, and finally be able to interpret the new readings in units we understand.[4]

Let's try following the same process Kepler used. Along the way, we'll use a tool he never had available: PyTorch!

5.2.2 Gathering some data

We'll start by making a note of temperature data in good old Celsius[5] and measurements from our new thermometer, and figure things out. After a couple of weeks, here's the data (code/p1ch5/1_parameter_estimation.ipynb):

[4] This task—fitting model outputs to continuous values in terms of the types discussed in chapter 4—is called a *regression* problem. In chapter 7 and part 2, we will be concerned with *classification* problems.

[5] The author of this chapter is Italian, so please forgive him for using sensible units.

```
# In[2]:
t_c = [0.5,  14.0, 15.0, 28.0, 11.0,  8.0,  3.0, -4.0,  6.0, 13.0, 21.0]
t_u = [35.7, 55.9, 58.2, 81.9, 56.3, 48.9, 33.9, 21.8, 48.4, 60.4, 68.4]
t_c = torch.tensor(t_c)
t_u = torch.tensor(t_u)
```

Here, the `t_c` values are temperatures in Celsius, and the `t_u` values are our unknown units. We can expect noise in both measurements, coming from the devices themselves and from our approximate readings. For convenience, we've already put the data into tensors; we'll use it in a minute.

5.2.3 Visualizing the data

A quick plot of our data in figure 5.3 tells us that it's noisy, but we think there's a pattern here.

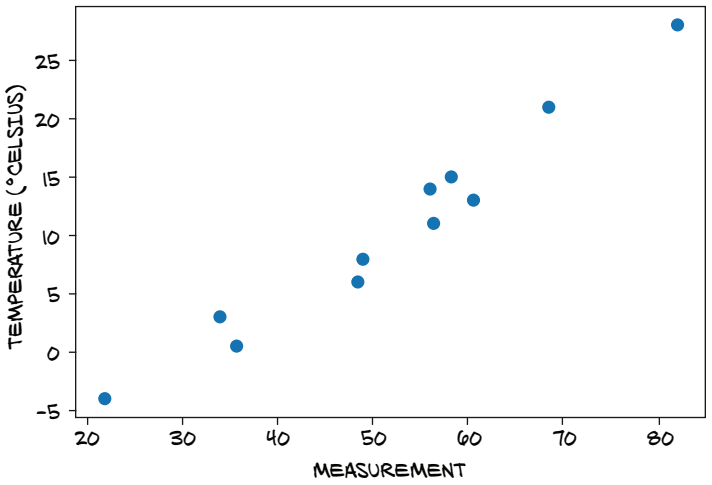


Figure 5.3 Our unknown data just might follow a linear model.

NOTE Spoiler alert: we know a linear model is correct because the problem and data have been fabricated, but please bear with us. It's a useful motivating example to build our understanding of what PyTorch is doing under the hood.

5.2.4 Choosing a linear model as a first try

In the absence of further knowledge, we assume the simplest possible model for converting between the two sets of measurements, just like Kepler might have done. The two may be linearly related—that is, multiplying `t_u` by a factor and adding a constant, we may get the temperature in Celsius (up to an error that we omit):

```
t_c = w * t_u + b
```

Is this a reasonable assumption? Probably; we'll see how well the final model performs. We chose to name `w` and `b` after *weight* and *bias*, two very common terms for linear scaling and the additive constant—we'll bump into those all the time.[6]

OK, now we need to estimate `w` and `b`, the parameters in our model, based on the data we have. We must do it so that temperatures we obtain from running the unknown temperatures `t_u` through the model are close to temperatures we actually measured in Celsius. If that sounds like fitting a line through a set of measurements, well, yes, because that's exactly what we're doing. We'll go through this simple example using PyTorch and realize that training a neural network will essentially involve changing the model for a slightly more elaborate one, with a few (or a metric ton) more parameters.

Let's flesh it out again: we have a model with some unknown parameters, and we need to estimate those parameters so that the error between predicted outputs and measured values is as low as possible. We notice that we still need to exactly define a measure of the error. Such a measure, which we refer to as the *loss function*, should be high if the error is high and should ideally be as low as possible for a perfect match. Our optimization process should therefore aim at finding `w` and `b` so that the loss function is at a minimum.

5.3 Less loss is what we want

A *loss function* (or *cost function*) is a function that computes a single numerical value that the learning process will attempt to minimize. The calculation of loss typically involves taking the difference between the desired outputs for some training samples and the outputs actually produced by the model when fed those samples. In our case, that would be the difference between the predicted temperatures `t_p` output by our model and the actual measurements: `t_p - t_c`.

We need to make sure the loss function makes the loss positive both when `t_p` is greater than and when it is less than the true `t_c`, since the goal is for `t_p` to match `t_c`. We have a few choices, the most straightforward being `|t_p - t_c|` and `(t_p - t_c)^2`. Based on the mathematical expression we choose, we can emphasize or discount certain errors. Conceptually, a loss function is a way of prioritizing which errors to fix from our training samples, so that our parameter updates result in adjustments to the outputs for the highly weighted samples instead of changes to some other samples' output that had a smaller loss.

Both of the example loss functions have a clear minimum at zero and grow monotonically as the predicted value moves further from the true value in either direction. Because the steepness of the growth also monotonically increases away from the minimum, both of them are said to be *convex*. Since our model is linear, the loss as a function of `w` and `b` is also convex.[7] Cases where the loss is a convex function of the model parameters are usually great to deal with because we can find a minimum very efficiently

[6] The weight tells us how much a given input influences the output. The bias is what the output would be if all inputs were zero.

[7] Contrast that with the function shown in figure 5.6, which is not convex.

through specialized algorithms. However, we will instead use less powerful but more generally applicable methods in this chapter. We do so because for the deep neural networks we are ultimately interested in, the loss is not a convex function of the inputs.

For our two loss functions `|t_p - t_c|` and `(t_p - t_c)^2`, as shown in figure 5.4, we notice that the square of the differences behaves more nicely around the minimum: the derivative of the error-squared loss with respect to `t_p` is zero when `t_p` equals `t_c`. The absolute value, on the other hand, has an undefined derivative right where we'd like to converge. This is less of an issue in practice than it looks like, but we'll stick to the square of differences for the time being.

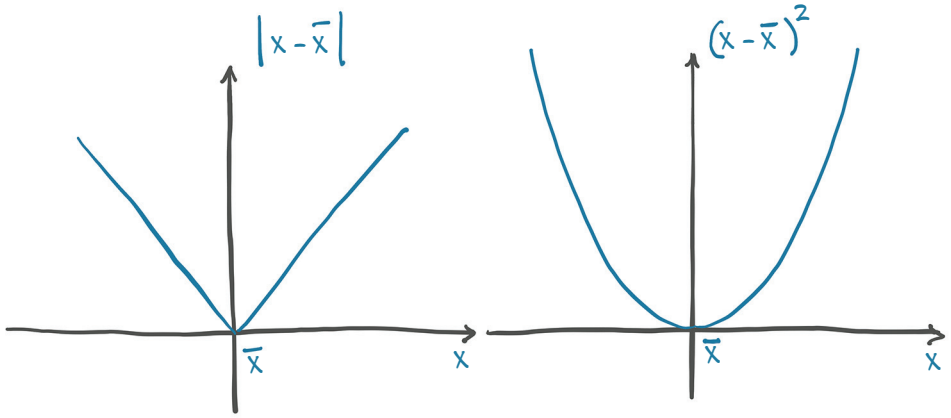


Figure 5.4 Absolute difference versus difference squared

It's worth noting that the square difference also penalizes wildly wrong results more than the absolute difference does. Often, having more slightly wrong results is better than having a few wildly wrong ones, and the squared difference helps prioritize those as desired.

5.3.1 From problem back to PyTorch

We've figured out the model and the loss function—we've already got a good part of the high-level picture in figure 5.2 figured out. Now we need to set the learning process in motion and feed it actual data. Also, enough with math notation; let's switch to PyTorch—after all, we came here for the *fun*.

We've already created our data tensors, so now let's write out the model as a Python function:

```
# In[3]:
def model(t_u, w, b):
    return w * t_u + b
```

We're expecting `t_u`, `w`, and `b` to be the input tensor, weight parameter, and bias parameter, respectively. In our model, the parameters will be PyTorch scalars (aka

zero-dimensional tensors), and the product operation will use broadcasting to yield the returned tensors. Anyway, time to define our loss:

```
# In[4]:
def loss_fn(t_p, t_c):
    squared_diffs = (t_p - t_c)**2
    return squared_diffs.mean()
```

Note that we are building a tensor of differences, taking their square element-wise, and finally producing a scalar loss function by averaging all of the elements in the resulting tensor. It is a *mean square loss*.

We can now initialize the parameters, invoke the model,

```
# In[5]:
w = torch.ones(())
b = torch.zeros(())

t_p = model(t_u, w, b)
t_p

# Out[5]:
tensor([35.7000, 55.9000, 58.2000, 81.9000, 56.3000, 48.9000, 33.9000,
        21.8000, 48.4000, 60.4000, 68.4000])
```

and check the value of the loss:

```
# In[6]:
loss = loss_fn(t_p, t_c)
loss

# Out[6]:
tensor(1763.8846)
```

We implemented the model and the loss in this section. We've finally reached the meat of the example: how do we estimate `w` and `b` such that the loss reaches a minimum? We'll first work things out by hand and then learn how to use PyTorch's superpowers to solve the same problem in a more general, off-the-shelf way.

Broadcasting

We mentioned broadcasting in chapter 3, and we promised to look at it more carefully when we need it. In our example, we have two scalars (zero-dimensional tensors) `w` and `b`, and we multiply them with and add them to vectors (one-dimensional tensors) of length *b*.

Usually—and in early versions of PyTorch, too—we can only use element-wise binary operations such as addition, subtraction, multiplication, and division for arguments of the same shape. The entries in matching positions in each of the tensors will be used to calculate the corresponding entry in the result tensor.

(continued)

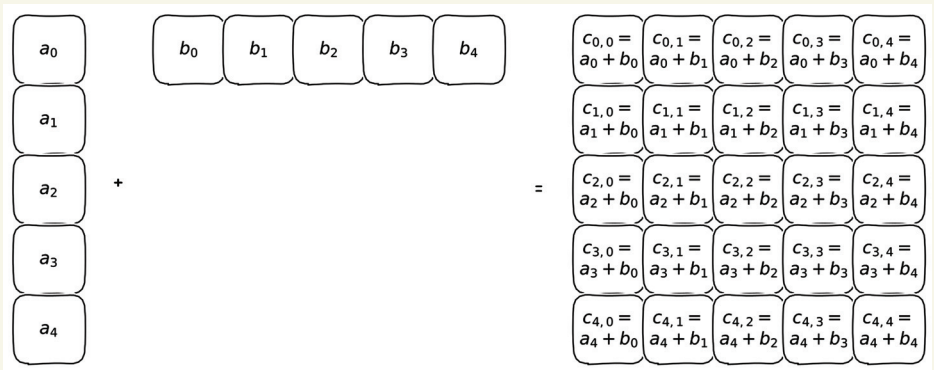
Broadcasting, which is popular in NumPy and adapted by PyTorch, relaxes this assumption for most binary operations. It uses the following rules to match tensor elements:

- For each index dimension, counted from the back, if one of the operands is size 1 in that dimension, PyTorch will use the single entry along this dimension with each of the entries in the other tensor along this dimension.
- If both sizes are greater than 1, they must be the same, and natural matching is used.
- If one of the tensors has more index dimensions than the other, the entirety of the other tensor will be used for each entry along these dimensions.

This sounds complicated (and it can be error-prone if we don't pay close attention, which is why we have named the tensor dimensions as shown in section 3.4), but usually, we can either write down the tensor dimensions to see what happens or picture what happens by using space dimensions to show the broadcasting, as in the following figure.

Of course, this would all be theory if we didn't have some code examples:

```
# In[7]:
x = torch.ones(())
y = torch.ones(3,1)
z = torch.ones(1,3)
a = torch.ones(2, 1, 1)
print(f"shapes: x: {x.shape}, y: {y.shape}")
```




```
print(f"        z: {z.shape}, a: {a.shape}")
print("x * y:", (x * y).shape)
print("y * z:", (y * z).shape)
print("y * z * a:", (y * z * a).shape)

# Out[7]:

shapes: x: torch.Size([]), y: torch.Size([3, 1])
        z: torch.Size([1, 3]), a: torch.Size([2, 1, 1])
x * y: torch.Size([3, 1])

y * z: torch.Size([3, 3])
y * z * a: torch.Size([2, 3, 3])
```

5.4 Down along the gradient

We'll optimize the loss function with respect to the parameters using the *gradient descent* algorithm. In this section, we'll build our intuition for how gradient descent works from first principles, which will help us a lot in the future. As we mentioned, there are ways to solve our example problem more efficiently, but those approaches aren't applicable to most deep learning tasks. Gradient descent is actually a very simple idea, and it scales up surprisingly well to large neural network models with millions of parameters.

Let's start with a mental image, which we conveniently sketched out in figure 5.5. Suppose we are in front of a machine sporting two knobs, labeled `w` and `b`. We are allowed to see the value of the loss on a screen, and we are told to minimize that value. Not knowing the effect of the knobs on the loss, we start fiddling with them and decide for each knob which direction makes the loss decrease. We decide to rotate both knobs in their direction of decreasing loss. Suppose we're far from the optimal value: we'd likely see the loss decrease quickly and then slow down as it gets closer to the minimum. We notice that at some point, the loss climbs back up again, so we invert the direction of rotation for one or both knobs. We also learn that when the loss changes slowly, it's a good idea to adjust the knobs more finely, to avoid reaching the point where the loss goes back up. After a while, eventually, we converge to a minimum.

Figure 5.5 A cartoon depiction of the optimization process, where a person with knobs for `w` and `b` searches for the direction to turn the knobs that makes the loss decrease

5.4.1 Decreasing loss

Gradient descent is not that different from the scenario we just described. The idea is to compute the rate of change of the loss with respect to each parameter, and modify each parameter in the direction of decreasing loss. Just like when we were fiddling with the knobs, we can estimate the rate of change by adding a small number to `w` and `b` and seeing how much the loss changes in that neighborhood:

```
# In[8]:
delta = 0.1

loss_rate_of_change_w = \
    (loss_fn(model(t_u, w + delta, b), t_c) -
     loss_fn(model(t_u, w - delta, b), t_c)) / (2.0 * delta)
```

This is saying that in the neighborhood of the current values of `w` and `b`, a unit increase in `w` leads to some change in the loss. If the change is negative, then we need to increase `w` to minimize the loss, whereas if the change is positive, we need to decrease `w`. By how much? Applying a change to `w` that is proportional to the rate of change of the loss is a good idea, especially when the loss has several parameters: we apply a change to those that exert a significant change on the loss. It is also wise to change the parameters slowly in general, because the rate of change could be dramatically different at a distance from the neighborhood of the current `w` value. Therefore, we typically should scale the rate of change by a small factor. This scaling factor has many names; the one we use in machine learning is `learning_rate`:

```
# In[9]:
learning_rate = 1e-2

w = w - learning_rate * loss_rate_of_change_w
```

We can do the same with `b`:

```
# In[10]:
loss_rate_of_change_b = \
    (loss_fn(model(t_u, w, b + delta), t_c) -
     loss_fn(model(t_u, w, b - delta), t_c)) / (2.0 * delta)

b = b - learning_rate * loss_rate_of_change_b
```

This represents the basic parameter-update step for gradient descent. By reiterating these evaluations (and provided we choose a small enough learning rate), we will converge to an optimal value of the parameters for which the loss computed on the given data is minimal. We'll show the complete iterative process soon, but the way we just computed our rates of change is rather crude and needs an upgrade before we move on. Let's see why and how.

5.4.2 Getting analytical

Computing the rate of change by using repeated evaluations of the model and loss in order to probe the behavior of the loss function in the neighborhood of `w` and `b` doesn't scale well to models with many parameters. Also, it is not always clear how large the neighborhood should be. We chose `delta` equal to 0.1 in the previous section, but it all depends on the shape of the loss as a function of `w` and `b`. If the loss changes too quickly compared to `delta`, we won't have a very good idea of in which direction the loss is decreasing the most.

What if we could make the neighborhood infinitesimally small, as in figure 5.6? That's exactly what happens when we analytically take the derivative of the loss with respect to a parameter. In a model with two or more parameters like the one we're dealing with, we compute the individual derivatives of the loss with respect to each parameter and put them in a vector of derivatives: the *gradient*.

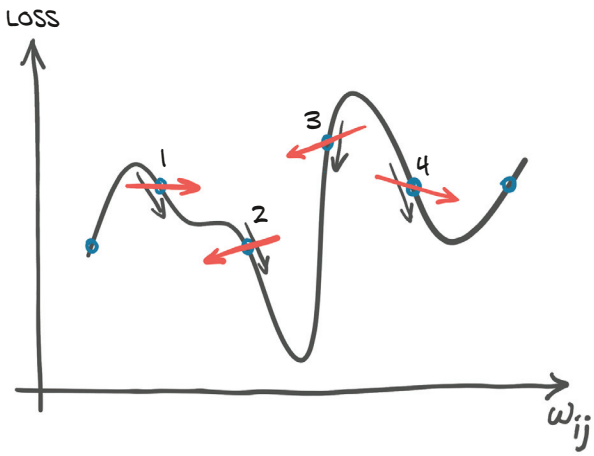


Figure 5.6 Differences in the estimated directions for descent when evaluating them at discrete locations versus analytically

Computing the derivatives

In order to compute the derivative of the loss with respect to a parameter, we can apply the chain rule and compute the derivative of the loss with respect to its input (which is the output of the model), times the derivative of the model with respect to the parameter:

```
d loss_fn / d w = (d loss_fn / d t_p) * (d t_p / d w)
```

Recall that our model is a linear function, and our loss is a sum of squares. Let's figure out the expressions for the derivatives. Recalling the expression for the loss:

```
# In[4]:
def loss_fn(t_p, t_c):
    squared_diffs = (t_p - t_c)**2
    return squared_diffs.mean()
```

Remembering that `d x^2 / d x = 2 x`, we get

```
# In[11]:
def dloss_fn(t_p, t_c):
    dsq_diffs = 2 * (t_p - t_c) / t_p.size(0)
    return dsq_diffs
```

The division is from the derivative of mean.

Applying the derivatives to the model

For the model, recalling that our model is

```
# In[3]:
def model(t_u, w, b):
    return w * t_u + b
```

we get these derivatives:

```
# In[12]:
def dmodel_dw(t_u, w, b):
    return t_u


# In[13]:
def dmodel_db(t_u, w, b):
    return 1.0
```

DEFINING THE GRADIENT FUNCTION

Putting all of this together, the function returning the gradient of the loss with respect to `w` and `b` is

```
# In[14]:
def grad_fn(t_u, t_c, t_p, w, b):
    dloss_dtp = dloss_fn(t_p, t_c)
    dloss_dw = dloss_dtp * dmodel_dw(t_u, w, b)
    dloss_db = dloss_dtp * dmodel_db(t_u, w, b)
    return torch.stack([dloss_dw.sum(), dloss_db.sum()])
```

The summation is the reverse of the broadcasting we implicitly do when applying the parameters to an entire vector of inputs in the model.

The same idea expressed in mathematical notation is shown in figure 5.7. Again, we're averaging (that is, summing and dividing by a constant) over all the data points to get a single scalar quantity for each partial derivative of the loss.

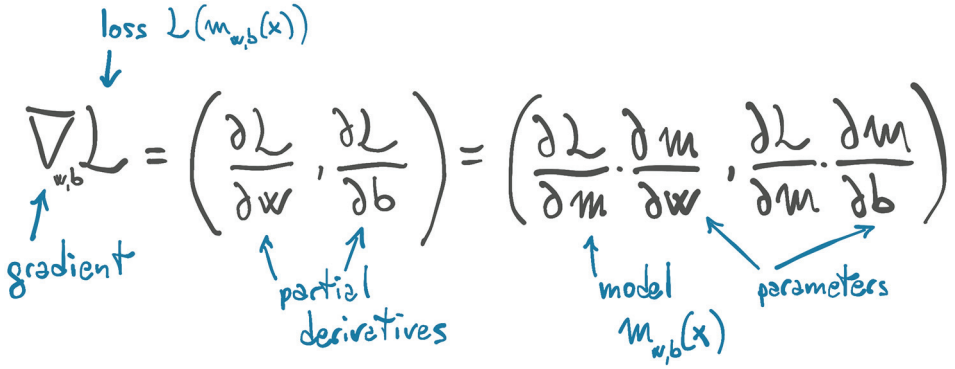


Figure 5.7 The derivative of the loss function with respect to the weights

5.4.3 *Iterating to fit the model*

We now have everything in place to optimize our parameters. Starting from a tentative value for a parameter, we can iteratively apply updates to it for a fixed number of iterations, or until `w` and `b` stop changing. There are several stopping criteria; for now, we'll stick to a fixed number of iterations.

THE TRAINING LOOP

Since we're at it, let's introduce another piece of terminology. We call a training iteration during which we update the parameters for all of our training samples an *epoch*.

The complete training loop looks like this (code/p1ch5/1_parameter_estimation.ipynb):

```
# In[15]:
def training_loop(n_epochs, learning_rate, params, t_u, t_c):
    for epoch in range(1, n_epochs + 1):
        w, b = params

        t_p = model(t_u, w, b)        <-- Forward pass
        loss = loss_fn(t_p, t_c)
        grad = grad_fn(t_u, t_c, t_p, w, b)     <-- Backward pass

        params = params - learning_rate * grad

        print('Epoch %d, Loss %f' % (epoch, float(loss)))   <-- This logging line can be very verbose.

    return params
```

The actual logging logic used for the output in this text is more complicated (see cell 15 in the same notebook: http://mng.bz/pBB8), but the differences are unimportant for understanding the core concepts in this chapter.

Now, let's invoke our training loop:

```
# In[17]:
training_loop(
    n_epochs = 100,
    learning_rate = 1e-2,
    params = torch.tensor([1.0, 0.0]),
    t_u = t_u,
    t_c = t_c)

# Out[17]:
Epoch 1, Loss 1763.884644
    Params: tensor([-44.1730,  -0.8260])
    Grad:   tensor([4517.2969,   82.6000])
Epoch 2, Loss 5802485.500000
    Params: tensor([2568.4014,   45.1637])
    Grad:   tensor([-261257.4219,   -4598.9712])
Epoch 3, Loss 19408035840.000000
    Params: tensor([-148527.7344,   -2616.3933])
    Grad:   tensor([15109614.0000,   266155.7188])
...
Epoch 10, Loss 90901154706620645225508955521810432.000000
    Params: tensor([3.2144e+17, 5.6621e+15])
    Grad:   tensor([-3.2700e+19, -5.7600e+17])
Epoch 11, Loss inf
    Params: tensor([-1.8590e+19, -3.2746e+17])
    Grad:   tensor([1.8912e+21, 3.3313e+19])

tensor([-1.8590e+19, -3.2746e+17])
```

OVERTRAINING

Wait, what happened? Our training process literally blew up, leading to losses becoming `inf`. This is a clear sign that `params` is receiving updates that are too large, and their values start oscillating back and forth as each update overshoots and the next overcorrects even more. The optimization process is unstable: it *diverges* instead of converging to a minimum. We want to see smaller and smaller updates to `params`, not larger, as shown in figure 5.8.

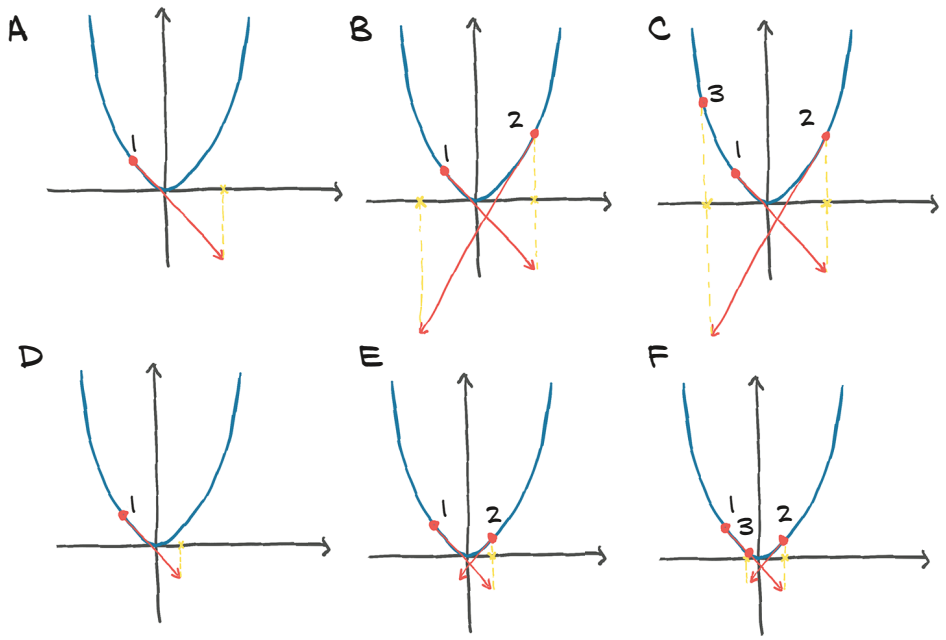


Figure 5.8 Top: Diverging optimization on a convex function (parabola-like) due to large steps. Bottom: Converging optimization with small steps.

How can we limit the magnitude of `learning_rate * grad`? Well, that looks easy. We could simply choose a smaller `learning_rate`, and indeed, the learning rate is one of the things we typically change when training does not go as well as we would like.[8] We usually change learning rates by orders of magnitude, so we might try with `1e-3` or `1e-4`, which would decrease the magnitude of the updates by orders of magnitude. Let's go with `1e-4` and see how it works out:

```
# In[18]:
training_loop(
    n_epochs = 100,
```

[8] The fancy name for this is *hyperparameter tuning*. *Hyperparameter* refers to the fact that we are training the model's parameters, but the hyperparameters control how this training goes. Typically these are more or less set manually. In particular, they cannot be part of the same optimization.

```
    learning_rate = 1e-4,
    params = torch.tensor([1.0, 0.0]),
    t_u = t_u,
    t_c = t_c)

# Out[18]:
Epoch 1, Loss 1763.884644
    Params: tensor([ 0.5483, -0.0083])
    Grad:   tensor([4517.2969,   82.6000])
Epoch 2, Loss 323.090546
    Params: tensor([ 0.3623, -0.0118])
    Grad:   tensor([1859.5493,   35.7843])
Epoch 3, Loss 78.929634
    Params: tensor([ 0.2858, -0.0135])
    Grad:   tensor([765.4667,  16.5122])
...
Epoch 10, Loss 29.105242
    Params: tensor([ 0.2324, -0.0166])
    Grad:   tensor([1.4803, 3.0544])
Epoch 11, Loss 29.104168
    Params: tensor([ 0.2323, -0.0169])
    Grad:   tensor([0.5781, 3.0384])
...
Epoch 99, Loss 29.023582
    Params: tensor([ 0.2327, -0.0435])
    Grad:   tensor([-0.0533,  3.0226])
Epoch 100, Loss 29.022669
    Params: tensor([ 0.2327, -0.0438])
    Grad:   tensor([-0.0532,  3.0226])

tensor([ 0.2327, -0.0438])
```

Nice—the behavior is now stable. But there's another problem: the updates to parameters are very small, so the loss decreases very slowly and eventually stalls. We could obviate this issue by making `learning_rate` adaptive: that is, change according to the magnitude of updates. There are optimization schemes that do that, and we'll see one toward the end of this chapter, in section 5.5.2.

However, there's another potential troublemaker in the update term: the gradient itself. Let's go back and look at `grad` at epoch 1 during optimization.

5.4.4 Normalizing inputs

We can see that the first-epoch gradient for the weight is about 50 times larger than the gradient for the bias. This means the weight and bias live in differently scaled spaces. If this is the case, a learning rate that's large enough to meaningfully update one will be so large as to be unstable for the other; and a rate that's appropriate for the other won't be large enough to meaningfully change the first. That means we're not going to be able to update our parameters unless we change something about our formulation of the problem. We could have individual learning rates for each parameter, but for models with many parameters, this would be too much to bother with; it's babysitting of the kind we don't like.

There's a simpler way to keep things in check: changing the inputs so that the gradients aren't quite so different. We can make sure the range of the input doesn't get too far from the range of –1.0 to 1.0, roughly speaking. In our case, we can achieve something close enough to that by simply multiplying `t_u` by 0.1:

```
# In[19]:
t_un = 0.1 * t_u
```

Here, we denote the normalized version of `t_u` by appending an `n` to the variable name. At this point, we can run the training loop on our normalized input:

```
# In[20]:
training_loop(
    n_epochs = 100,
    learning_rate = 1e-2,
    params = torch.tensor([1.0, 0.0]),
    t_u = t_un,
    t_c = t_c)

# Out[20]:
Epoch 1, Loss 80.364342
    Params: tensor([1.7761, 0.1064])
    Grad:   tensor([-77.6140, -10.6400])
Epoch 2, Loss 37.574917
    Params: tensor([2.0848, 0.1303])
    Grad:   tensor([-30.8623,  -2.3864])
Epoch 3, Loss 30.871077
    Params: tensor([2.2094, 0.1217])
    Grad:   tensor([-12.4631,   0.8587])
...
Epoch 10, Loss 29.030487
    Params: tensor([ 2.3232, -0.0710])
    Grad:   tensor([-0.5355,  2.9295])
Epoch 11, Loss 28.941875
    Params: tensor([ 2.3284, -0.1003])
    Grad:   tensor([-0.5240,  2.9264])
...
Epoch 99, Loss 22.214186
    Params: tensor([ 2.7508, -2.4910])
    Grad:   tensor([-0.4453,  2.5208])
Epoch 100, Loss 22.148710
    Params: tensor([ 2.7553, -2.5162])
    Grad:   tensor([-0.4446,  2.5165])

tensor([ 2.7553, -2.5162])
```

We've updated t_u to our new, rescaled t_un.

Even though we set our learning rate back to `1e-2`, parameters don't blow up during iterative updates. Let's take a look at the gradients: they're of similar magnitude, so using a single `learning_rate` for both parameters works just fine. We could probably do a better job of normalization than a simple rescaling by a factor of 10, but since doing so is good enough for our needs, we're going to stick with that for now.

NOTE The normalization here absolutely helps get the network trained, but you could make an argument that it's not strictly needed to optimize the parameters for this particular problem. That's absolutely true! This problem is small enough that there are numerous ways to beat the parameters into submission. However, for larger, more sophisticated problems, normalization is an easy and effective (if not crucial!) tool to use to improve model convergence.

Let's run the loop for enough iterations to see the changes in `params` get small. We'll change `n_epochs` to 5,000:

```
# In[21]:
params = training_loop(
    n_epochs = 5000,
    learning_rate = 1e-2,
    params = torch.tensor([1.0, 0.0]),
    t_u = t_un,
    t_c = t_c,
    print_params = False)

params

# Out[21]:
Epoch 1, Loss 80.364342
Epoch 2, Loss 37.574917
Epoch 3, Loss 30.871077
...
Epoch 10, Loss 29.030487
Epoch 11, Loss 28.941875
...
Epoch 99, Loss 22.214186
Epoch 100, Loss 22.148710
...
Epoch 4000, Loss 2.927680
Epoch 5000, Loss 2.927648

tensor([  5.3671, -17.3012])
```

Good: our loss decreases while we change parameters along the direction of gradient descent. It doesn't go exactly to zero; this could mean there aren't enough iterations to converge to zero, or that the data points don't sit exactly on a line. As we anticipated, our measurements were not perfectly accurate, or there was noise involved in the reading.

But look: the values for `w` and `b` look an awful lot like the numbers we need to use to convert Celsius to Fahrenheit (after accounting for our earlier normalization when we multiplied our inputs by 0.1). The exact values would be `w=5.5556` and `b=-17.7778`. Our fancy thermometer was showing temperatures in Fahrenheit the whole time. No big discovery, except that our gradient descent optimization process works!

5.4.5 Visualizing (again)

Let's revisit something we did right at the start: plotting our data. Seriously, this is the first thing anyone doing data science should do. Always plot the heck out of the data:

```
# In[22]:
%matplotlib inline
from matplotlib import pyplot as plt

t_p = model(t_un, *params)

fig = plt.figure(dpi=600)
plt.xlabel("Temperature (°Fahrenheit)")
plt.ylabel("Temperature (°Celsius)")
plt.plot(t_u.numpy(), t_p.detach().numpy())
plt.plot(t_u.numpy(), t_c.numpy(), 'o')
```

Remember that we're training on the normalized unknown units. We also use argument unpacking.

But we're plotting the raw unknown values.

We are using a Python trick called *argument unpacking* here: `*params` means to pass the elements of `params` as individual arguments. In Python, this is usually done with lists or tuples, but we can also use argument unpacking with PyTorch tensors, which are split along the leading dimension. So here, `model(t_un, *params)` is equivalent to `model(t_un, params[0], params[1])`.

This code produces figure 5.9. Our linear model is a good model for the data, it seems. It also seems our measurements are somewhat erratic. We should either call our optometrist for a new pair of glasses or think about returning our fancy thermometer.

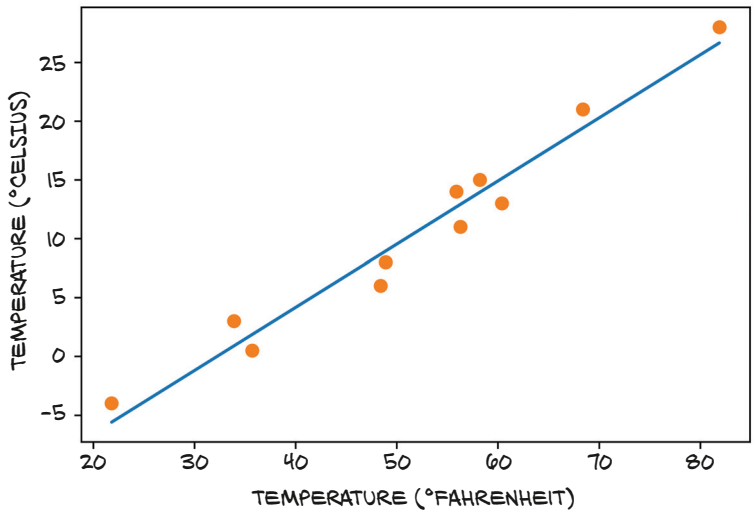


Figure 5.9 The plot of our linear-fit model (solid line) versus our input data (circles)

5.5 PyTorch's autograd: Backpropagating all things

In our little adventure, we just saw a simple example of backpropagation: we computed the gradient of a composition of functions—the model and the loss—with respect to their innermost parameters (`w` and `b`) by propagating derivatives backward using the *chain rule*. The basic requirement here is that all functions we're dealing with can be differentiated analytically. If this is the case, we can compute the gradient—what we earlier called "the rate of change of the loss"—with respect to the parameters in one sweep.

Even if we have a complicated model with millions of parameters, as long as our model is differentiable, computing the gradient of the loss with respect to the parameters amounts to writing the analytical expression for the derivatives and evaluating them *once*. Granted, writing the analytical expression for the derivatives of a very deep composition of linear and nonlinear functions is not a lot of fun.[9] It isn't particularly quick, either.

5.5.1 Computing the gradient automatically

This is when PyTorch tensors come to the rescue, with a PyTorch component called *autograd*. Chapter 3 presented a comprehensive overview of what tensors are and what functions we can call on them. We left out one very interesting aspect, however: PyTorch tensors can remember where they come from, in terms of the operations and parent tensors that originated them, and they can automatically provide the chain of derivatives of such operations with respect to their inputs. This means we won't need to derive our model by hand;[10] given a forward expression, no matter how nested, PyTorch will automatically provide the gradient of that expression with respect to its input parameters.

APPLYING AUTOGRAD

At this point, the best way to proceed is to rewrite our thermometer calibration code, this time using autograd, and see what happens. First, we recall our model and loss function.

Listing 5.1 code/p1ch5/2_autograd.ipynb

```
# In[3]:
def model(t_u, w, b):
    return w * t_u + b

# In[4]:
def loss_fn(t_p, t_c):
    squared_diffs = (t_p - t_c)**2
    return squared_diffs.mean()
```

[9] Or maybe it is; we won't judge how you spend your weekend!
[10] Bummer! What are we going to do on Saturdays, now?

Let's again initialize a parameters tensor:

```
# In[5]:
params = torch.tensor([1.0, 0.0], requires_grad=True)
```

USING THE GRAD ATTRIBUTE

Notice the `requires_grad=True` argument to the tensor constructor? That argument is telling PyTorch to track the entire family tree of tensors resulting from operations on `params`. In other words, any tensor that will have `params` as an ancestor will have access to the chain of functions that were called to get from `params` to that tensor. In case these functions are differentiable (and most PyTorch tensor operations will be), the value of the derivative will be automatically populated as a `grad` attribute of the `params` tensor.

In general, all PyTorch tensors have an attribute named `grad`. Normally, it's `None`:

```
# In[6]:
params.grad is None

# Out[6]:
True
```

All we have to do to populate it is to start with a tensor with `requires_grad` set to `True`, then call the model and compute the loss, and then call `backward` on the `loss` tensor:

```
# In[7]:
loss = loss_fn(model(t_u, *params), t_c)
loss.backward()

params.grad

# Out[7]:
tensor([4517.2969,   82.6000])
```

At this point, the `grad` attribute of `params` contains the derivatives of the loss with respect to each element of params.

When we compute our `loss` while the parameters `w` and `b` require gradients, in addition to performing the actual computation, PyTorch creates the autograd graph with the operations (in black circles) as nodes, as shown in the top row of figure 5.10. When we call `loss.backward()`, PyTorch traverses this graph in the reverse direction to compute the gradients, as shown by the arrows in the bottom row of the figure.

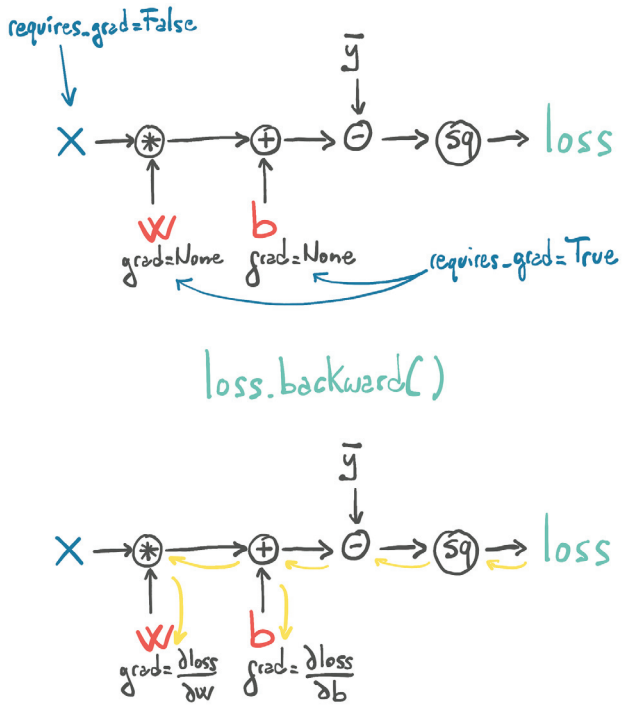


Figure 5.10 The forward graph and backward graph of the model as computed with autograd

ACCUMULATING GRAD FUNCTIONS

We could have any number of tensors with `requires_grad` set to `True` and any composition of functions. In this case, PyTorch would compute the derivatives of the loss throughout the chain of functions (the computation graph) and accumulate their values in the `grad` attribute of those tensors (the leaf nodes of the graph).

Alert! *Big gotcha ahead.* This is something PyTorch newcomers—and a lot of more experienced folks, too—trip up on regularly. We just wrote *accumulate*, not *store*.

WARNING Calling `backward` will lead derivatives to *accumulate* at leaf nodes. We need to *zero the gradient explicitly* after using it for parameter updates.

Let's repeat together: calling `backward` will lead derivatives to *accumulate* at leaf nodes. So if `backward` was called earlier, the loss is evaluated again, `backward` is called again (as in any training loop), and the gradient at each leaf is accumulated (that is, summed) on top of the one computed at the previous iteration, which leads to an incorrect value for the gradient.

In order to prevent this from occurring, we need to *zero the gradient explicitly* at each iteration. We can do this easily using the in-place `zero_` method:

```
# In[8]:
if params.grad is not None:
    params.grad.zero_()
```

NOTE You might be curious why zeroing the gradient is a required step instead of zeroing happening automatically whenever we call `backward`. Doing it this way provides more flexibility and control when working with gradients in complicated models.

Having this reminder drilled into our heads, let's see what our autograd-enabled training code looks like, start to finish:

```
# In[9]:
def training_loop(n_epochs, learning_rate, params, t_u, t_c):
    for epoch in range(1, n_epochs + 1):
        if params.grad is not None:
            params.grad.zero_()

        t_p = model(t_u, *params)
        loss = loss_fn(t_p, t_c)
        loss.backward()

        with torch.no_grad():
            params -= learning_rate * params.grad

        if epoch % 500 == 0:
            print('Epoch %d, Loss %f' % (epoch, float(loss)))

    return params
```

This could be done at any point in the loop prior to calling loss.backward().

This is a somewhat cumbersome bit of code, but as we'll see in the next section, it's not an issue in practice.

Note that our code updating `params` is not quite as straightforward as we might have expected. There are two particularities. First, we are encapsulating the update in a `no_grad` context using the Python `with` statement. This means within the `with` block, the PyTorch autograd mechanism should *look away*:[11] that is, not add edges to the forward graph. In fact, when we are executing this bit of code, the forward graph that PyTorch records is consumed when we call `backward`, leaving us with the `params` leaf node. But now we want to change this leaf node before we start building a fresh forward graph on top of it. While this use case is usually wrapped inside the optimizers we discuss in section 5.5.2, we will take a closer look when we see another common use of `no_grad` in section 5.5.4.

Second, we update `params` in place. This means we keep the same `params` tensor around but subtract our update from it. When using autograd, we usually avoid in-place updates because PyTorch's autograd engine might need the values we would be modifying for the backward pass. Here, however, we are operating without autograd, and it is beneficial to keep the `params` tensor. Not replacing the parameters by assigning new tensors to their variable name will become crucial when we register our parameters with the optimizer in section 5.5.2.

[11] In reality, it will track that something changed params using an in-place operation.

Let's see if it works:

```
# In[10]:
training_loop(
    n_epochs = 5000,
    learning_rate = 1e-2,
    params = torch.tensor([1.0, 0.0], requires_grad=True),
    t_u = t_un,
    t_c = t_c)
```

Adding requires_grad=True is key.

Again, we're using the normalized t_un instead of t_u.

```
# Out[10]:
Epoch 500, Loss 7.860116
Epoch 1000, Loss 3.828538
Epoch 1500, Loss 3.092191
Epoch 2000, Loss 2.957697
Epoch 2500, Loss 2.933134
Epoch 3000, Loss 2.928648
Epoch 3500, Loss 2.927830
Epoch 4000, Loss 2.927679
Epoch 4500, Loss 2.927652
Epoch 5000, Loss 2.927647

tensor([  5.3671, -17.3012], requires_grad=True)
```

The result is the same as we got previously. Good for us! It means that while we are *capable* of computing derivatives by hand, we no longer need to.

5.5.2 Optimizers a la carte

In the example code, we used *vanilla* gradient descent for optimization, which worked fine for our simple case. Needless to say, there are several optimization strategies and tricks that can assist convergence, especially when models get complicated.

We'll dive deeper into this topic in later chapters, but now is the right time to introduce the way PyTorch abstracts the optimization strategy away from user code: that is, the training loop we've examined. This saves us from the boilerplate busywork of having to update each and every parameter to our model ourselves. The `torch` module has an `optim` submodule where we can find classes implementing different optimization algorithms. Here's an abridged list (code/p1ch5/3_optimizers.ipynb):

```
# In[5]:
import torch.optim as optim

dir(optim)

# Out[5]:
['ASGD',
 'Adadelta',
 'Adagrad',
 'Adam',
 'Adamax',
 'LBFGS',
 'Optimizer',
```

```
 'RMSprop',
 'Rprop',
 'SGD',
 'SparseAdam',
...
]
```

Every optimizer constructor takes a list of parameters (aka PyTorch tensors, typically with `requires_grad` set to `True`) as the first input. All parameters passed to the optimizer are retained inside the optimizer object so the optimizer can update their values and access their `grad` attribute, as represented in figure 5.11.

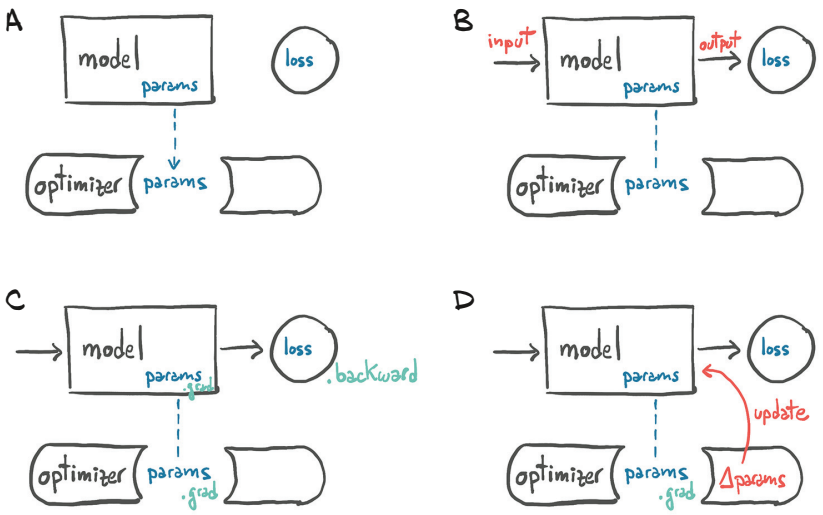


Figure 5.11 (A) Conceptual representation of how an optimizer holds a reference to parameters. (B) After a loss is computed from inputs, (C) a call to `.backward` leads to `.grad` being populated on parameters. (D) At that point, the optimizer can access `.grad` and compute the parameter updates.

Each optimizer exposes two methods: `zero_grad` and `step`. `zero_grad` zeroes the `grad` attribute of all the parameters passed to the optimizer upon construction. `step` updates the value of those parameters according to the optimization strategy implemented by the specific optimizer.

USING A GRADIENT DESCENT OPTIMIZER

Let's create `params` and instantiate a gradient descent optimizer:

```
# In[6]:
params = torch.tensor([1.0, 0.0], requires_grad=True)
learning_rate = 1e-5
optimizer = optim.SGD([params], lr=learning_rate)
```

Here SGD stands for *stochastic gradient descent*. Actually, the optimizer itself is exactly a vanilla gradient descent (as long as the `momentum` argument is set to `0.0`, which is the default). The term *stochastic* comes from the fact that the gradient is typically obtained by averaging over a random subset of all input samples, called a *minibatch*. However, the optimizer does not know if the loss was evaluated on all the samples (vanilla) or a random subset of them (stochastic), so the algorithm is literally the same in the two cases.

Anyway, let's take our fancy new optimizer for a spin:

```
# In[7]:
t_p = model(t_u, *params)
loss = loss_fn(t_p, t_c)
loss.backward()

optimizer.step()

params

# Out[7]:
tensor([ 9.5483e-01, -8.2600e-04], requires_grad=True)
```

The value of `params` is updated upon calling `step` without us having to touch it ourselves! What happens is that the optimizer looks into `params.grad` and updates `params`, subtracting `learning_rate` times `grad` from it, exactly as in our former hand-rolled code.

Ready to stick this code in a training loop? Nope! The big gotcha almost got us—we forgot to zero out the gradients. Had we called the previous code in a loop, gradients would have accumulated in the leaves at every call to `backward`, and our gradient descent would have been all over the place! Here's the loop-ready code, with the extra `zero_grad` at the correct spot (right before the call to `backward`):

```
# In[8]:
params = torch.tensor([1.0, 0.0], requires_grad=True)
learning_rate = 1e-2
optimizer = optim.SGD([params], lr=learning_rate)

t_p = model(t_un, *params)
loss = loss_fn(t_p, t_c)

optimizer.zero_grad()
loss.backward()
optimizer.step()

params

# Out[8]:
tensor([1.7761, 0.1064], requires_grad=True)
```

As before, the exact placement of this call is somewhat arbitrary. It could be earlier in the loop as well.

Perfect! See how the `optim` module helps us abstract away the specific optimization scheme? All we have to do is provide a list of params to it (that list can be extremely

long, as is needed for very deep neural network models), and we can forget about the details.

Let's update our training loop accordingly:

```
# In[9]:
def training_loop(n_epochs, optimizer, params, t_u, t_c):
    for epoch in range(1, n_epochs + 1):
        t_p = model(t_u, *params)
        loss = loss_fn(t_p, t_c)

        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        if epoch % 500 == 0:
            print('Epoch %d, Loss %f' % (epoch, float(loss)))

    return params

# In[10]:
params = torch.tensor([1.0, 0.0], requires_grad=True)
learning_rate = 1e-2
optimizer = optim.SGD([params], lr=learning_rate)

training_loop(
    n_epochs = 5000,
    optimizer = optimizer,
    params = params,
    t_u = t_un,
    t_c = t_c)

# Out[10]:
Epoch 500, Loss 7.860118
Epoch 1000, Loss 3.828538
Epoch 1500, Loss 3.092191
Epoch 2000, Loss 2.957697
Epoch 2500, Loss 2.933134
Epoch 3000, Loss 2.928648
Epoch 3500, Loss 2.927830
Epoch 4000, Loss 2.927680
Epoch 4500, Loss 2.927651
Epoch 5000, Loss 2.927648

tensor([  5.3671, -17.3012], requires_grad=True)
```

It's important that both params are the same object; otherwise the optimizer won't know what parameters were used by the model.

Again, we get the same result as before. Great: this is further confirmation that we know how to descend a gradient by hand!

TESTING OTHER OPTIMIZERS

In order to test more optimizers, all we have to do is instantiate a different optimizer, say `Adam`, instead of `SGD`. The rest of the code stays as it is. Pretty handy stuff.

We won't go into much detail about Adam; suffice to say that it is a more sophisticated optimizer in which the learning rate is set adaptively. In addition, it is a lot less sensitive to the scaling of the parameters—so insensitive that we can go back to using

the original (non-normalized) input `t_u`, and even increase the learning rate to `1e-1`, and Adam won't even blink:

```
# In[11]:
params = torch.tensor([1.0, 0.0], requires_grad=True)
learning_rate = 1e-1
optimizer = optim.Adam([params], lr=learning_rate)    <-- New optimizer class

training_loop(
    n_epochs = 2000,
    optimizer = optimizer,
    params = params,
    t_u = t_u,        <-- We're back to the original t_u as our input.
    t_c = t_c)

# Out[11]:
Epoch 500, Loss 7.612903
Epoch 1000, Loss 3.086700
Epoch 1500, Loss 2.928578
Epoch 2000, Loss 2.927646

tensor([  0.5367, -17.3021], requires_grad=True)
```

The optimizer is not the only flexible part of our training loop. Let's turn our attention to the model. In order to train a neural network on the same data and the same loss, all we would need to change is the `model` function. It wouldn't make particular sense in this case, since we know that converting Celsius to Fahrenheit amounts to a linear transformation, but we'll do it anyway in chapter 6. We'll see quite soon that neural networks allow us to remove our arbitrary assumptions about the shape of the function we should be approximating. Even so, we'll see how neural networks manage to be trained even when the underlying processes are highly nonlinear (such in the case of describing an image with a sentence, as we saw in chapter 2).

We have touched on a lot of the essential concepts that will enable us to train complicated deep learning models while knowing what's going on under the hood: backpropagation to estimate gradients, autograd, and optimizing weights of models using gradient descent or other optimizers. Really, there isn't a lot more. The rest is mostly filling in the blanks, however extensive they are.

Next up, we're going to offer an aside on how to split our samples, because that sets up a perfect use case for learning how to better control autograd.

5.5.3 Training, validation, and overfitting

Johannes Kepler taught us one last thing that we didn't discuss so far, remember? He kept part of the data on the side so that he could validate his models on independent observations. This is a vital thing to do, especially when the model we adopt could potentially approximate functions of any shape, as in the case of neural networks. In other words, a highly adaptable model will tend to use its many parameters to make sure the loss is minimal *at* the data points, but we'll have no guarantee that the model

behaves well *away from* or *in between* the data points. After all, that's what we're asking the optimizer to do: minimize the loss *at* the data points. Sure enough, if we had independent data points that we didn't use to evaluate our loss or descend along its negative gradient, we would soon find out that evaluating the loss at those independent data points would yield higher-than-expected loss. We have already mentioned this phenomenon, called *overfitting*.

The first action we can take to combat overfitting is recognizing that it might happen. In order to do so, as Kepler figured out in 1600, we must take a few data points out of our dataset (the *validation set*) and only fit our model on the remaining data points (the *training set*), as shown in figure 5.12. Then, while we're fitting the model, we can evaluate the loss once on the training set and once on the validation set. When we're trying to decide if we've done a good job of fitting our model to the data, we must look at both!

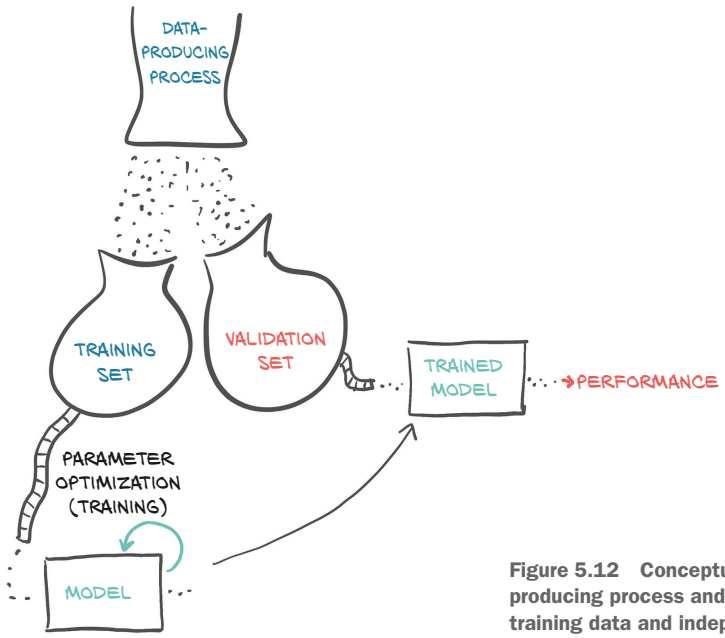


Figure 5.12 Conceptual representation of a data-producing process and the collection and use of training data and independent validation data

EVALUATING THE TRAINING LOSS

The training loss will tell us if our model can fit the training set at all—in other words, if our model has enough *capacity* to process the relevant information in the data. If our mysterious thermometer somehow managed to measure temperatures using a logarithmic scale, our poor linear model would not have had a chance to fit those measurements and provide us with a sensible conversion to Celsius. In that case, our training loss (the loss we were printing in the training loop) would stop decreasing well before approaching zero.

A deep neural network can potentially approximate complicated functions, provided that the number of neurons, and therefore parameters, is high enough. The fewer the number of parameters, the simpler the shape of the function our network will be able to approximate. So, rule 1: if the training loss is not decreasing, chances are the model is too simple for the data. The other possibility is that our data just doesn't contain meaningful information that lets it explain the output: if the nice folks at the shop sell us a barometer instead of a thermometer, we will have little chance of predicting temperature in Celsius from just pressure, even if we use the latest neural network architecture from Quebec (www.umontreal.ca/en/artificialintelligence).

Generalizing to the validation set

What about the validation set? Well, if the loss evaluated in the validation set doesn't decrease along with the training set, it means our model is improving its fit of the samples it is seeing during training, but it is not *generalizing* to samples outside this precise set. As soon as we evaluate the model at new, previously unseen points, the values of the loss function are poor. So, rule 2: if the training loss and the validation loss diverge, we're overfitting.

Let's delve into this phenomenon a little, going back to our thermometer example. We could have decided to fit the data with a more complicated function, like a piecewise polynomial or a really large neural network. It could generate a model meandering its way through the data points, as in figure 5.13, just because it pushes the loss very close to zero. Since the behavior of the function away from the data points does not increase the loss, there's nothing to keep the model in check for inputs away from the training data points.

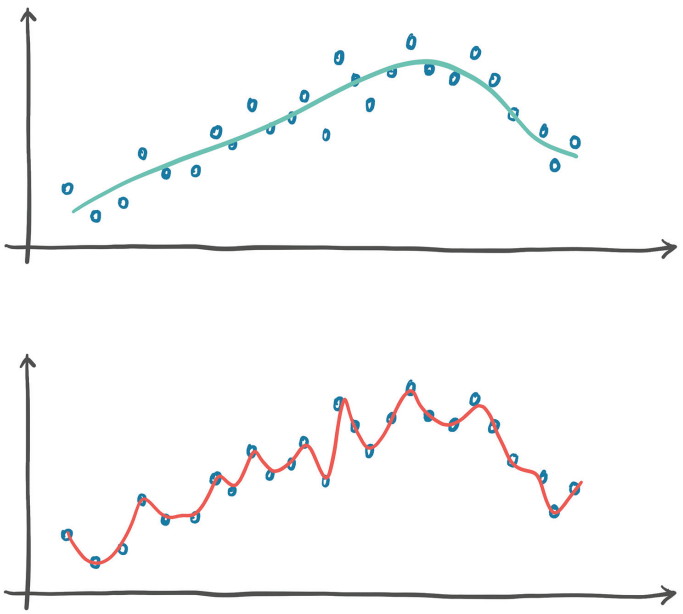


Figure 5.13 Rather extreme example of overfitting

What's the cure, though? Good question. From what we just said, overfitting really looks like a problem of making sure the behavior of the model *in between* data points is sensible for the process we're trying to approximate. First of all, we should make sure we get enough data for the process. If we collected data from a sinusoidal process by sampling it regularly at a low frequency, we would have a hard time fitting a model to it.

Assuming we have enough data points, we should make sure the model that is capable of fitting the training data is as regular as possible in between them. There are several ways to achieve this. One is adding *penalization terms* to the loss function, to make it cheaper for the model to behave more smoothly and change more slowly (up to a point). Another is to add noise to the input samples, to artificially create new data points in between training data samples and force the model to try to fit those, too. There are several other ways, all of them somewhat related to these. But the best favor we can do to ourselves, at least as a first move, is to make our model simpler. From an intuitive standpoint, a simpler model may not fit the training data as perfectly as a more complicated model would, but it will likely behave more regularly in between data points.

We've got some nice trade-offs here. On the one hand, we need the model to have enough capacity for it to fit the training set. On the other, we need the model to avoid overfitting. Therefore, in order to choose the right size for a neural network model in terms of parameters, the process is based on two steps: increase the size until it fits, and then scale it down until it stops overfitting.

We'll see more about this in chapter 12—we'll discover that our life will be a balancing act between fitting and overfitting. For now, let's get back to our example and see how we can split the data into a training set and a validation set. We'll do it by shuffling `t_u` and `t_c` the same way and then splitting the resulting shuffled tensors into two parts.

SPLITTING A DATASET

Shuffling the elements of a tensor amounts to finding a permutation of its indices. The `randperm` function does exactly this:

```
# In[12]:
n_samples = t_u.shape[0]
n_val = int(0.2 * n_samples)

shuffled_indices = torch.randperm(n_samples)

train_indices = shuffled_indices[:-n_val]
val_indices = shuffled_indices[-n_val:]

train_indices, val_indices

# Out[12]:
(tensor([9, 6, 5, 8, 4, 7, 0, 1, 3]), tensor([ 2, 10]))
```

Since these are random, don't be surprised if your values end up different from here on out.

We just got index tensors that we can use to build training and validation sets starting from the data tensors:

```
# In[13]:
train_t_u = t_u[train_indices]
train_t_c = t_c[train_indices]

val_t_u = t_u[val_indices]
val_t_c = t_c[val_indices]

train_t_un = 0.1 * train_t_u
val_t_un = 0.1 * val_t_u
```

Our training loop doesn't really change. We just want to additionally evaluate the validation loss at every epoch, to have a chance to recognize whether we're overfitting:

```
# In[14]:
def training_loop(n_epochs, optimizer, params, train_t_u, val_t_u,
                  train_t_c, val_t_c):
    for epoch in range(1, n_epochs + 1):
        train_t_p = model(train_t_u, *params)
        train_loss = loss_fn(train_t_p, train_t_c)

        val_t_p = model(val_t_u, *params)
        val_loss = loss_fn(val_t_p, val_t_c)

        optimizer.zero_grad()
        train_loss.backward()
        optimizer.step()

        if epoch <= 3 or epoch % 500 == 0:
            print(f"Epoch {epoch}, Training loss {train_loss.item():.4f},"
                  f" Validation loss {val_loss.item():.4f}")

    return params
```

These two pairs of lines are the same except for the train_* vs. val_* inputs.

Note that there is no val_loss.backward() here, since we don't want to train the model on the validation data.

```
# In[15]:
params = torch.tensor([1.0, 0.0], requires_grad=True)
learning_rate = 1e-2
optimizer = optim.SGD([params], lr=learning_rate)

training_loop(
    n_epochs = 3000,
    optimizer = optimizer,
    params = params,
    train_t_u = train_t_un,
    val_t_u = val_t_un,
    train_t_c = train_t_c,
    val_t_c = val_t_c)
```

Since we're using SGD again, we're back to using normalized inputs.

```
# Out[15]:
Epoch 1, Training loss 66.5811, Validation loss 142.3890
Epoch 2, Training loss 38.8626, Validation loss 64.0434
Epoch 3, Training loss 33.3475, Validation loss 39.4590
Epoch 500, Training loss 7.1454, Validation loss 9.1252
```

```
Epoch 1000, Training loss 3.5940, Validation loss 5.3110
Epoch 1500, Training loss 3.0942, Validation loss 4.1611
Epoch 2000, Training loss 3.0238, Validation loss 3.7693
Epoch 2500, Training loss 3.0139, Validation loss 3.6279
Epoch 3000, Training loss 3.0125, Validation loss 3.5756

tensor([  5.1964, -16.7512], requires_grad=True)
```

Here we are not being entirely fair to our model. The validation set is really small, so the validation loss will only be meaningful up to a point. In any case, we note that the validation loss is higher than our training loss, although not by an order of magnitude. We expect a model to perform better on the training set, since the model parameters are being shaped by the training set. Our main goal is to also see both the training loss *and* the validation loss decreasing. While ideally both losses would be roughly the same value, as long as the validation loss stays reasonably close to the training loss, we know that our model is continuing to learn generalized things about our data. In figure 5.14, case C is ideal, while D is acceptable. In case A, the model isn't learning at all; and in case B, we see overfitting. We'll see more meaningful examples of overfitting in chapter 12.

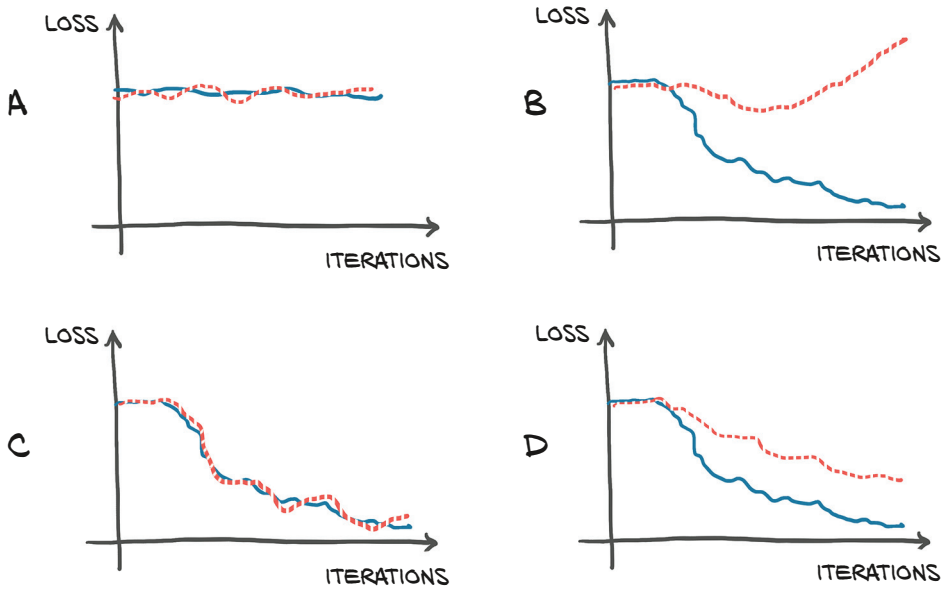


Figure 5.14 Overfitting scenarios when looking at the training (solid line) and validation (dotted line) losses. (A) Training and validation losses do not decrease; the model is not learning due to no information in the data or insufficient capacity of the model. (B) Training loss decreases while validation loss increases: overfitting. (C) Training and validation losses decrease exactly in tandem. Performance may be improved further as the model is not at the limit of overfitting. (D) Training and validation losses have different absolute values but similar trends: overfitting is under control.

5.5.4 Autograd nits and switching it off

From the previous training loop, we can appreciate that we only ever call `backward` on `train_loss`. Therefore, errors will only ever backpropagate based on the training set—the validation set is used to provide an independent evaluation of the accuracy of the model's output on data that wasn't used for training.

The curious reader will have an embryo of a question at this point. The model is evaluated twice—once on `train_t_u` and once on `val_t_u`—and then `backward` is called. Won't this confuse autograd? Won't `backward` be influenced by the values generated during the pass on the validation set?

Luckily for us, this isn't the case. The first line in the training loop evaluates `model` on `train_t_u` to produce `train_t_p`. Then `train_loss` is evaluated from `train_t_p`. This creates a computation graph that links `train_t_u` to `train_t_p` to `train_loss`. When `model` is evaluated again on `val_t_u`, it produces `val_t_p` and `val_loss`. In this case, a separate computation graph will be created that links `val_t_u` to `val_t_p` to `val_loss`. Separate tensors have been run through the same functions, `model` and `loss_fn`, generating separate computation graphs, as shown in figure 5.15.

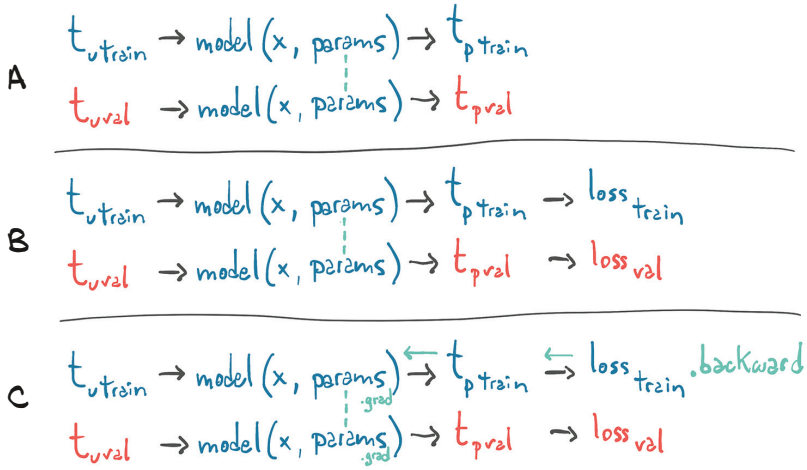


Figure 5.15 Diagram showing how gradients propagate through a graph with two losses when `.backward` is called on one of them

The only tensors these two graphs have in common are the parameters. When we call `backward` on `train_loss`, we run `backward` on the first graph. In other words, we accumulate the derivatives of `train_loss` with respect to the parameters based on the computation generated from `train_t_u`.

If we (incorrectly) called `backward` on `val_loss` as well, we would accumulate the derivatives of `val_loss` with respect to the parameters *on the same leaf nodes*. Remember the `zero_grad` thing, whereby gradients are accumulated on top of each other every time we call `backward` unless we zero out the gradients explicitly? Well, here something

very similar would happen: calling `backward` on `val_loss` would lead to gradients accumulating in the `params` tensor, on top of those generated during the `train_loss.backward()` call. In this case, we would effectively train our model on the whole dataset (both training and validation), since the gradient would depend on both. Pretty interesting.

There's another element for discussion here. Since we're not ever calling `backward` on `val_loss`, why are we building the graph in the first place? We could in fact just call `model` and `loss_fn` as plain functions, without tracking the computation. However optimized, building the autograd graph comes with additional costs that we could totally forgo during the validation pass, especially when the model has millions of parameters.

In order to address this, PyTorch allows us to switch off autograd when we don't need it, using the `torch.no_grad` context manager.[12] We won't see any meaningful advantage in terms of speed or memory consumption on our small problem. However, for larger models, the differences can add up. We can make sure this works by checking the value of the `requires_grad` attribute on the `val_loss` tensor:

```
# In[16]:
def training_loop(n_epochs, optimizer, params, train_t_u, val_t_u,
                  train_t_c, val_t_c):
    for epoch in range(1, n_epochs + 1):
        train_t_p = model(train_t_u, *params)
        train_loss = loss_fn(train_t_p, train_t_c)

        with torch.no_grad():
            val_t_p = model(val_t_u, *params)
            val_loss = loss_fn(val_t_p, val_t_c)
            assert val_loss.requires_grad == False

        optimizer.zero_grad()
        train_loss.backward()
        optimizer.step()
```

Context manager here

Checks that our output requires_grad args are forced to False inside this block

Using the related `set_grad_enabled` context, we can also condition the code to run with `autograd` enabled or disabled, according to a Boolean expression—typically indicating whether we are running in training or inference mode. We could, for instance, define a `calc_forward` function that takes data as input and runs `model` and `loss_fn` with or without autograd according to a Boolean `train_is` argument:

```
# In[17]:
def calc_forward(t_u, t_c, is_train):
    with torch.set_grad_enabled(is_train):
        t_p = model(t_u, *params)
        loss = loss_fn(t_p, t_c)
    return loss
```

[12] We should not think that using `torch.no_grad` necessarily implies that the outputs do not require gradients. There are particular circumstances (involving views, as discussed in section 3.8.1) in which `requires_grad` is not set to `False` even when created in a `no_grad` context. It is best to use the `detach` function if we need to be sure.

5.6 Conclusion

We started this chapter with a big question: how is it that a machine can learn from examples? We spent the rest of the chapter describing the mechanism with which a model can be optimized to fit data. We chose to stick with a simple model in order to see all the moving parts without unneeded complications.

Now that we've had our fill of appetizers, in chapter 6 we'll finally get to the main course: using a neural network to fit our data. We'll work on solving the same thermometer problem, but with the more powerful tools provided by the `torch.nn` module. We'll adopt the same spirit of using this small problem to illustrate the larger uses of PyTorch. The problem doesn't need a neural network to reach a solution, but it will allow us to develop a simpler understanding of what's required to train a neural network.

5.7 Exercise

1. Redefine the model to be `w2 * t_u ** 2 + w1 * t_u + b`.
   a. What parts of the training loop, and so on, need to change to accommodate this redefinition?
   b. What parts are agnostic to swapping out the model?
   c. Is the resulting loss higher or lower after training?
   d. Is the actual result better or worse?

5.8 Summary

- Linear models are the simplest reasonable model to use to fit data.
- Convex optimization techniques can be used for linear models, but they do not generalize to neural networks, so we focus on stochastic gradient descent for parameter estimation.
- Deep learning can be used for generic models that are not engineered for solving a specific task, but instead can be automatically adapted to specialize themselves on the problem at hand.
- Learning algorithms amount to optimizing parameters of models based on observations. A loss function is a measure of the error in carrying out a task, such as the error between predicted outputs and measured values. The goal is to get the loss function as low as possible.
- The rate of change of the loss function with respect to the model parameters can be used to update the same parameters in the direction of decreasing loss.
- The `optim` module in PyTorch provides a collection of ready-to-use optimizers for updating parameters and minimizing loss functions.
- Optimizers use the autograd feature of PyTorch to compute the gradient for each parameter, depending on how that parameter contributes to the final output. This allows users to rely on the dynamic computation graph during complex forward passes.

- Context managers like `with torch.no_grad():` can be used to control autograd's behavior.
- Data is often split into separate sets of training samples and validation samples. This lets us evaluate a model on data it was not trained on.
- Overfitting a model happens when the model's performance continues to improve on the training set but degrades on the validation set. This is usually due to the model not generalizing, and instead memorizing the desired outputs for the training set.

6 Using a neural network to fit the data

This chapter covers

- Nonlinear activation functions as the key difference compared with linear models
- Working with PyTorch's `nn` module
- Solving a linear-fit problem with a neural network

So far, we've taken a close look at how a linear model can learn and how to make that happen in PyTorch. We've focused on a very simple regression problem that used a linear model with only one input and one output. Such a simple example allowed us to dissect the mechanics of a model that learns, without getting overly distracted by the implementation of the model itself. As we saw in the overview diagram in chapter 5, figure 5.2 (repeated here as figure 6.1), the exact details of a model are not needed to understand the high-level process that trains the model. Backpropagating errors to parameters and then updating those parameters by taking the gradient with respect to the loss is the same no matter what the underlying model is.

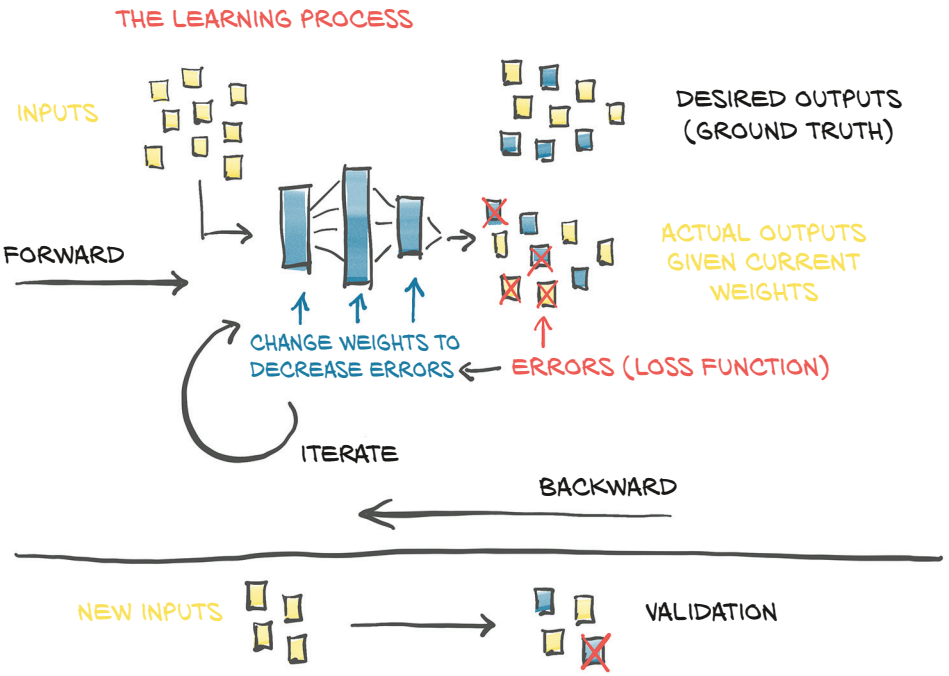


Figure 6.1 Our mental model of the learning process, as implemented in chapter 5

In this chapter, we will make some changes to our model architecture: we're going to implement a full artificial neural network to solve our temperature-conversion problem. We'll continue using our training loop from the last chapter, along with our Fahrenheit-to-Celsius samples split into training and validation sets. We could start to use a quadratic model: rewriting `model` as a quadratic function of its input (for example, `y = a * x**2 + b * x + c`). Since such a model would be differentiable, PyTorch would take care of computing gradients, and the training loop would work as usual. That wouldn't be too interesting for us, though, because we would still be fixing the shape of the function.

This is the chapter where we begin to hook together the foundational work we've put in and the PyTorch features you'll be using day in and day out as you work on your projects. You'll gain an understanding of what's going on underneath the porcelain of the PyTorch API, rather than it just being so much black magic. Before we get into the implementation of our new model, though, let's cover what we mean by *artificial neural network*.

6.1 Artificial neurons

At the core of deep learning are neural networks: mathematical entities capable of representing complicated functions through a composition of simpler functions. The term *neural network* is obviously suggestive of a link to the way our brain works. As a

matter of fact, although the initial models were inspired by neuroscience,[1] modern artificial neural networks bear only a slight resemblance to the mechanisms of neurons in the brain. It seems likely that both artificial and physiological neural networks use vaguely similar mathematical strategies for approximating complicated functions because that family of strategies works very effectively.

> **NOTE** We are going to drop the *artificial* and refer to these constructs as just *neural networks* from here forward.

The basic building block of these complicated functions is the *neuron*, as illustrated in figure 6.2. At its core, it is nothing but a linear transformation of the input (for example, multiplying the input by a number [the *weight*] and adding a constant [the *bias*]) followed by the application of a fixed nonlinear function (referred to as the *activation function*).

Mathematically, we can write this out as $o = f(w * x + b)$, with x as our input, w our weight or scaling factor, and b as our bias or offset. f is our activation function, set to the hyperbolic tangent, or `tanh` function here. In general, x and, hence, o can be simple scalars, or vector-valued (meaning holding many scalar values); and similarly, w

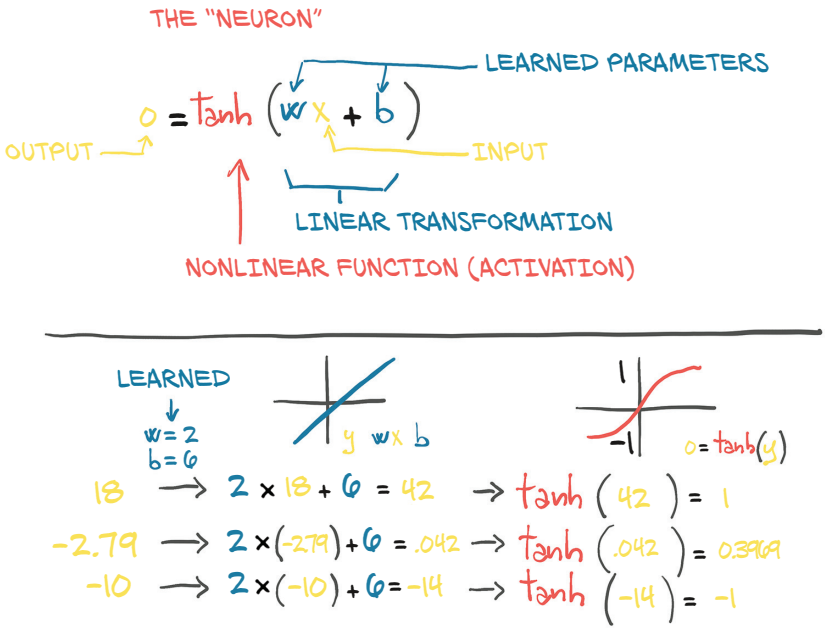


Figure 6.2 An artificial neuron: a linear transformation enclosed in a nonlinear function

[1] See F. Rosenblatt, "The Perceptron: A Probabilistic Model for Information Storage and Organization in the Brain," *Psychological Review* 65(6), 386–408 (1958), https://pubmed.ncbi.nlm.nih.gov/13602029/.

can be a single scalar or matrix, while *b* is a scalar or vector (the dimensionality of the inputs and weights must match, however). In the latter case, the previous expression is referred to as a *layer* of neurons, since it represents many neurons via the multidimensional weights and biases.

6.1.1 Composing a multilayer network

A multilayer neural network, as represented in figure 6.3, is made up of a composition of functions like those we just discussed

```
x_1 = f(w_0 * x + b_0)
x_2 = f(w_1 * x_1 + b_1)
...
y = f(w_n * x_n + b_n)
```

where the output of a layer of neurons is used as an input for the following layer. Remember that `w_0` here is a matrix, and `x` is a vector! Using a vector allows `w_0` to hold an entire *layer* of neurons, not just a single weight.

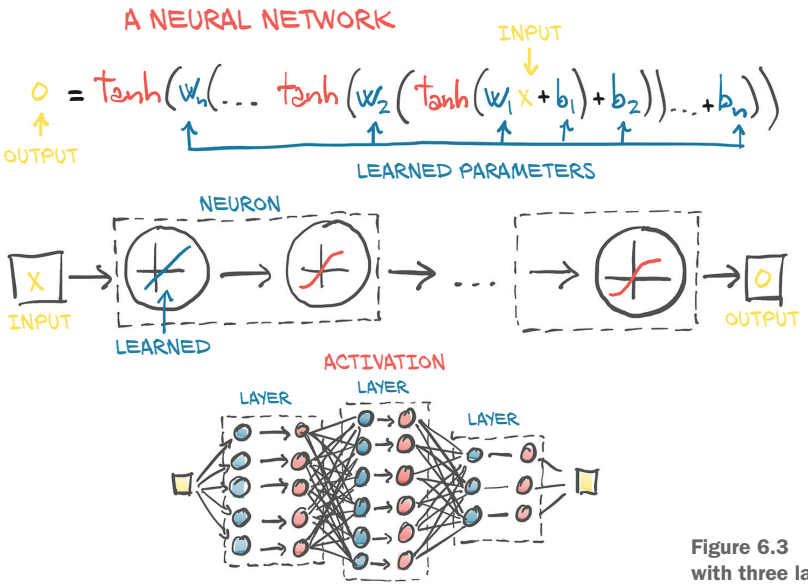


Figure 6.3 A neural network with three layers

6.1.2 Understanding the error function

An important difference between our earlier linear model and what we'll actually be using for deep learning is the shape of the error function. Our linear model and error-squared loss function had a convex error curve with a singular, clearly defined minimum. If we were to use other methods, we could solve for the parameters minimizing the error function automatically and definitively. That means that our parameter updates were attempting to *estimate* that singular correct answer as best they could.

Neural networks do not have that same property of a convex error surface, even when using the same error-squared loss function! There's no single right answer for each parameter we're attempting to approximate. Instead, we are trying to get all of the parameters, when acting *in concert*, to produce a useful output. Since that useful output is only going to *approximate* the truth, there will be some level of imperfection. Where and how imperfections manifest is somewhat arbitrary, and by implication the parameters that control the output (and, hence, the imperfections) are somewhat arbitrary as well. This results in neural network training looking very much like parameter estimation from a mechanical perspective, but we must remember that the theoretical underpinnings are quite different.

A big part of the reason neural networks have non-convex error surfaces is due to the activation function. The ability of an ensemble of neurons to approximate a very wide range of useful functions depends on the combination of the linear and nonlinear behavior inherent to each neuron.

6.1.3 All we need is activation

As we have seen, the simplest unit in (deep) neural networks is a linear operation (scaling + offset) followed by an activation function. We already had our linear operation in our latest model—the linear operation *was* the entire model. The activation function plays two important roles:

- In the inner parts of the model, it allows the output function to have different slopes at different values—something a linear function by definition cannot do. By trickily composing these differently sloped parts for many outputs, neural networks can approximate arbitrary functions, as we will see in section 6.1.6.[2]
- At the last layer of the network, it has the role of concentrating the outputs of the preceding linear operation into a given range.

Let's talk about what the second point means. Pretend that we're assigning a "good doggo" score to images. Pictures of retrievers and spaniels should have a high score, while images of airplanes and garbage trucks should have a low score. Bear pictures should have a lowish score, too, although higher than garbage trucks.

The problem is, we have to define a "high score": we've got the entire range of `float32` to work with, and that means we can go pretty high. Even if we say "it's a 10-point scale," there's still the issue that sometimes our model is going to produce a score of 11 out of 10. Remember that under the hood, it's all sums of (`w*x+b`) matrix multiplications, and those won't naturally limit themselves to a specific range of outputs.

---

[2] For an intuitive appreciation of this universal approximation property, you can pick a function from figure 6.5 and then build a building-block function that is almost zero in most parts and positive around $x = 0$ from scaled (including multiplied by negative numbers) and translated copies of the activation function. With scaled, translated, and dilated (squeezed along the *X*-axis) copies of this building-block function, you can then approximate any (continuous) function. In figure 6.6 the function in the middle row to the right could be such a building block. Michael Nielsen has an interactive demonstration in his online book *Neural Networks and Deep Learning* at http://mng.bz/Mdon.

CAPPING THE OUTPUT RANGE

We want to firmly constrain the output of our linear operation to a specific range so that the consumer of this output doesn't have to handle numerical inputs of puppies at 12/10, bears at –10, and garbage trucks at –1,000.

One possibility is to just cap the output values: anything below 0 is set to 0, and anything above 10 is set to 10. That's a simple activation function called `torch.nn.Hardtanh` (https://pytorch.org/docs/stable/nn.html#hardtanh, but note that the default range is –1 to +1).

COMPRESSING THE OUTPUT RANGE

Another family of functions that work well is `torch.nn.Sigmoid`, which includes `1 / (1 + e ** -x)`, `torch.tanh`, and others that we'll see in a moment. These functions have a curve that asymptotically approaches 0 or –1 as *x* goes to negative infinity, approaches 1 as *x* increases, and have a mostly constant slope at *x* == *0*. Conceptually, functions shaped this way work well because there's an area in the middle of our linear function's output that our neuron (which, again, is just a linear function followed by an activation) will be sensitive to, while everything else gets lumped next to the boundary values. As we can see in figure 6.4, our garbage truck gets a score of –0.97, while bears and foxes and wolves end up somewhere in the –0.3 to 0.3 range.

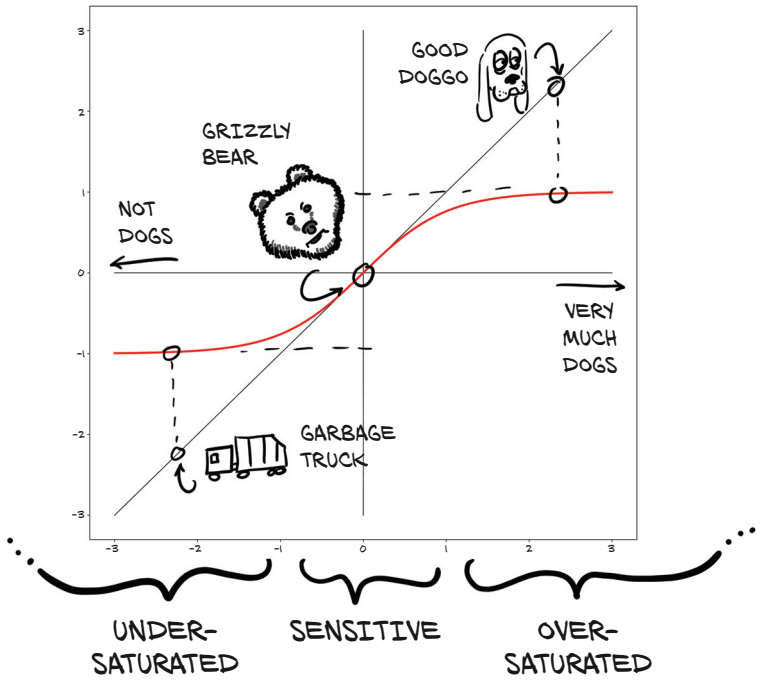


Figure 6.4 Dogs, bears, and garbage trucks being mapped to how dog-like they are via the `tanh` activation function

This results in garbage trucks being flagged as "not dogs," our good dog mapping to "clearly a dog," and our bear ending up somewhere in the middle. In code, we can see the exact values:

```
>>> import math
>>> math.tanh(-2.2)      <-- Garbage truck
-0.9757431300314515
>>> math.tanh(0.1)         <-- Bear
0.09966799462495582
>>> math.tanh(2.5)       <-- Good doggo
0.9866142981514303
```

With the bear in the sensitive range, small changes to the bear will result in a noticeable change to the result. For example, we could switch from a grizzly to a polar bear (which has a vaguely more traditionally canine face) and see a jump up the *Y*-axis as we slide toward the "very much a dog" end of the graph. Conversely, a koala bear would register as less dog-like, and we would see a drop in the activated output. There isn't much we could do to the garbage truck to make it register as dog-like, though: even with drastic changes, we might only see a shift from –0.97 to –0.8 or so.

6.1.4 More activation functions

There are quite a few activation functions, some of which are shown in figure 6.5. In the first column, we see the smooth functions `Tanh` and `Softplus`, while the second column has "hard" versions of the activation functions to their left: `Hardtanh` and `ReLU`. `ReLU` (for *rectified linear unit*) deserves special note, as it is currently considered

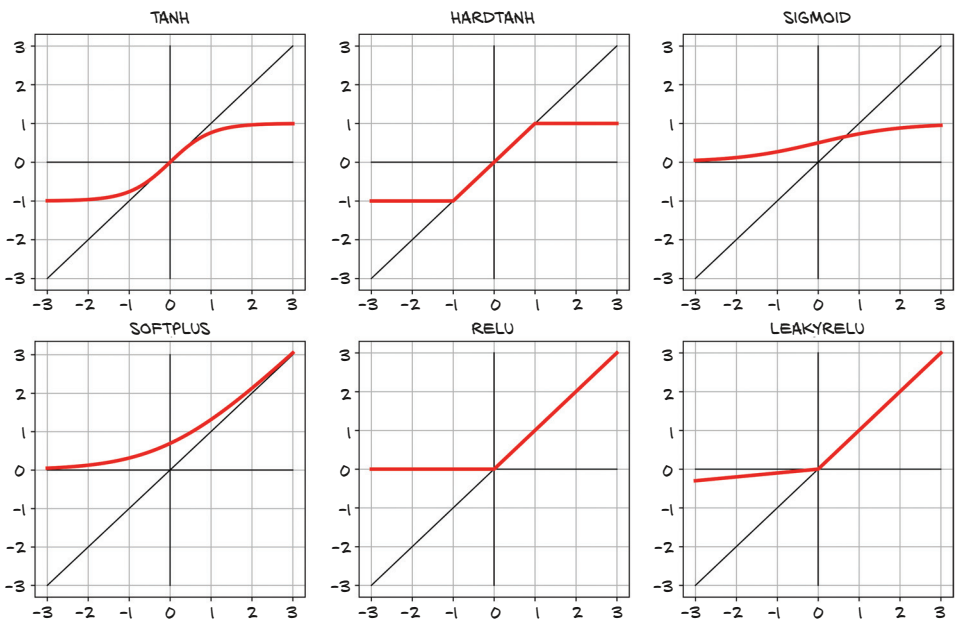


Figure 6.5 A collection of common and not-so-common activation functions

one of the best-performing general activation functions; many state-of-the-art results have used it. The `Sigmoid` activation function, also known as the *logistic function*, was widely used in early deep learning work but has since fallen out of common use except where we explicitly want to move to the 0…1 range: for example, when the output should be a probability. Finally, the `LeakyReLU` function modifies the standard `ReLU` to have a small positive slope, rather than being strictly zero for negative inputs (typically this slope is 0.01, but it's shown here with slope 0.1 for clarity).

6.1.5 Choosing the best activation function

Activation functions are curious, because with such a wide variety of proven successful ones (many more than shown in figure 6.5), it's clear that there are few, if any, strict requirements. As such, we're going to discuss some generalities about activation functions that can probably be trivially disproved in the specific. That said, by definition,[3] activation functions

- Are nonlinear. Repeated applications of (`w*x+b`) without an activation function results in a function of the same (affine linear) form. The nonlinearity allows the overall network to approximate more complex functions.
- Are differentiable, so that gradients can be computed through them. Point discontinuities, as we can see in `Hardtanh` or `ReLU`, are fine.

Without these characteristics, the network either falls back to being a linear model or becomes difficult to train.

The following are true for the functions:

- They have at least one sensitive range, where nontrivial changes to the input result in a corresponding nontrivial change to the output. This is needed for training.
- Many of them have an insensitive (or saturated) range, where changes to the input result in little or no change to the output.

By way of example, the `Hardtanh` function could easily be used to make piecewise-linear approximations of a function by combining the sensitive range with different weights and biases on the input.

Often (but far from universally so), the activation function will have at least one of these:

- A lower bound that is approached (or met) as the input goes to negative infinity
- A similar-but-inverse upper bound for positive infinity

Thinking of what we know about how backpropagation works, we can figure out that the errors will propagate backward through the activation more effectively when the inputs are in the response range, while errors will not greatly affect neurons for which

[3] Of course, even these statements aren't *always* true; see Jakob Foerster, "Nonlinear Computation in Deep Linear Networks," OpenAI, 2019, http://mng.bz/gygE.

the input is saturated (since the gradient will be close to zero, due to the flat area around the output).

Put together, all this results in a pretty powerful mechanism: we're saying that in a network built out of linear + activation units, when different inputs are presented to the network, (a) different units will respond in different ranges for the same inputs, and (b) the errors associated with those inputs will primarily affect the neurons operating in the sensitive range, leaving other units more or less unaffected by the learning process. In addition, thanks to the fact that derivatives of the activation with respect to its inputs are often close to 1 in the sensitive range, estimating the parameters of the linear transformation through gradient descent for the units that operate in that range will look a lot like the linear fit we have seen previously.

We are starting to get a deeper intuition for how joining many linear + activation units in parallel and stacking them one after the other leads us to a mathematical object that is capable of approximating complicated functions. Different combinations of units will respond to inputs in different ranges, and those parameters for those units are relatively easy to optimize through gradient descent, since learning will behave a lot like that of a linear function until the output saturates.

6.1.6 What learning means for a neural network

Building models out of stacks of linear transformations followed by differentiable activations leads to models that can approximate highly nonlinear processes and whose parameters we can estimate surprisingly well through gradient descent. This remains true even when dealing with models with millions of parameters. What makes using deep neural networks so attractive is that it saves us from worrying too much about the exact function that represents our data—whether it is quadratic, piecewise polynomial, or something else. With a deep neural network model, we have a universal approximator and a method to estimate its parameters. This approximator can be customized to our needs, in terms of model capacity and its ability to model complicated input/output relationships, just by composing simple building blocks. We can see some examples of this in figure 6.6.

The four upper-left graphs show four neurons—A, B, C, and D—each with its own (arbitrarily chosen) weight and bias. Each neuron uses the `Tanh` activation function with a min of –1 and a max of 1. The varied weights and biases move the center point and change how drastically the transition from min to max happens, but they clearly all have the same general shape. The columns to the right of those show both pairs of neurons added together (A + B and then C + D). Here, we start to see some interesting properties that mimic a single layer of neurons. A + B shows a slight *S* curve, with the extremes approaching 0, but both a positive bump and a negative bump in the middle. Conversely, C + D has only a large positive bump, which peaks at a higher value than our single-neuron max of 1.

In the third row, we begin to compose our neurons as they would be in a two-layer network. Both C(A + B) and D(A + B) have the same positive and negative bumps that A + B shows, but the positive peak is more subtle. The composition of C(A + B) + D(A + B)

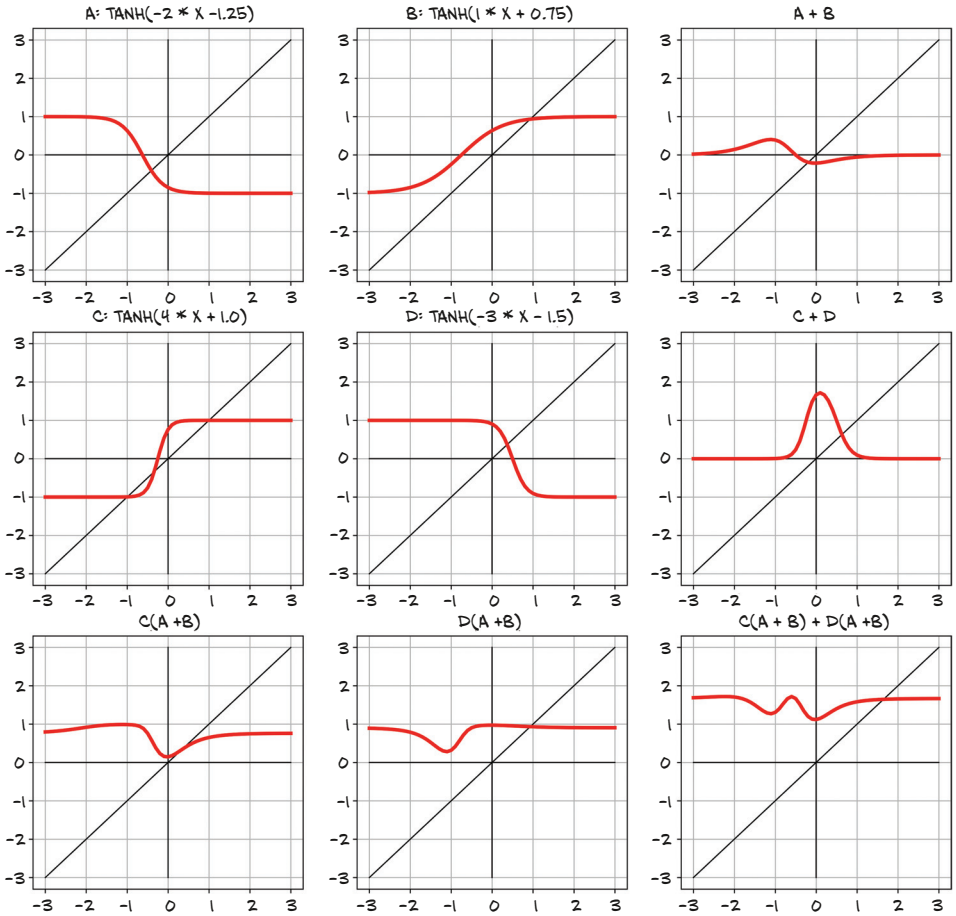


Figure 6.6 Composing multiple linear units and `tanh` activation functions to produce nonlinear outputs

shows a new property: *two* clearly negative bumps, and possibly a very subtle second positive peak as well, to the left of the main area of interest. All this with only four neurons in two layers!

Again, these neurons' parameters were chosen only to have a visually interesting result. Training consists of finding acceptable values for these weights and biases so that the resulting network correctly carries out a task, such as predicting likely temperatures given geographic coordinates and time of the year. By *carrying out a task successfully*, we mean obtaining a correct output on unseen data produced by the same data-generating process used for training data. A successfully trained network, through the values of its weights and biases, will capture the inherent structure of the data in the form of meaningful numerical representations that work correctly for previously unseen data.

Let's take another step in our realization of the mechanics of learning: deep neural networks give us the ability to approximate highly nonlinear phenomena without having an explicit model for them. Instead, starting from a generic, untrained model, we specialize it on a task by providing it with a set of inputs and outputs and a loss function from which to backpropagate. Specializing a generic model to a task using examples is what we refer to as *learning*, because the model wasn't built with that specific task in mind—no rules describing how that task worked were encoded in the model.

For our thermometer example, we assumed that both thermometers measured temperatures linearly. That assumption is where we implicitly encoded a rule for our task: we hardcoded the shape of our input/output function; we couldn't have approximated anything other than data points sitting around a line. As the dimensionality of a problem grows (that is, many inputs to many outputs) and input/output relationships get complicated, assuming a shape for the input/output function is unlikely to work. The job of a physicist or an applied mathematician is often to come up with a functional description of a phenomenon from first principles, so that we can estimate the unknown parameters from measurements and get an accurate model of the world. Deep neural networks, on the other hand, are families of functions that have the ability to approximate a wide range of input/output relationships without necessarily requiring us to come up with an explanatory model of a phenomenon. In a way, we're renouncing an explanation in exchange for the possibility of tackling increasingly complicated problems. In another way, we sometimes lack the ability, information, or computational resources to build an explicit model of what we're presented with, so data-driven methods are our only way forward.

6.2 The PyTorch nn module

All this talking about neural networks is probably making you really curious about building one from scratch with PyTorch. Our first step will be to replace our linear model with a neural network unit. This will be a somewhat useless step backward from a correctness perspective, since we've already verified that our calibration only required a linear function, but it will still be instrumental for starting on a sufficiently simple problem and scaling up later.

PyTorch has a whole submodule dedicated to neural networks, called `torch.nn`. It contains the building blocks needed to create all sorts of neural network architectures. Those building blocks are called *modules* in PyTorch parlance (such building blocks are often referred to as *layers* in other frameworks). A PyTorch module is a Python class deriving from the `nn.Module` base class. A module can have one or more `Parameter` instances as attributes, which are tensors whose values are optimized during the training process (think `w` and `b` in our linear model). A module can also have one or more submodules (subclasses of `nn.Module`) as attributes, and it will be able to track their parameters as well.

NOTE The submodules must be top-level *attributes*, not buried inside `list` or `dict` instances! Otherwise, the optimizer will not be able to locate the submodules (and, hence, their parameters). For situations where your model requires a list or dict of submodules, PyTorch provides `nn.ModuleList` and `nn.ModuleDict`.

Unsurprisingly, we can find a subclass of `nn.Module` called `nn.Linear`, which applies an affine transformation to its input (via the parameter attributes `weight` and `bias`) and is equivalent to what we implemented earlier in our thermometer experiments. We'll now start precisely where we left off and convert our previous code to a form that uses `nn`.

6.2.1 Using __call__ rather than forward

All PyTorch-provided subclasses of `nn.Module` have their `__call__` method defined. This allows us to instantiate an `nn.Linear` and call it as if it was a function, like so (code/p1ch6/1_neural_networks.ipynb):

```
# In[5]:
import torch.nn as nn
linear_model = nn.Linear(1, 1)
linear_model(t_un_val)

# Out[5]:
tensor([[0.6018],
        [0.2877]], grad_fn=<AddmmBackward>)
```

We'll look into the constructor arguments in a moment.

Calling an instance of `nn.Module` with a set of arguments ends up calling a method named `forward` with the same arguments. The `forward` method is what executes the forward computation, while `__call__` does other rather important chores before and after calling `forward`. So, it is technically possible to call `forward` directly, and it will produce the same output as `__call__`, but this should not be done from user code:

```
y = model(x)
y = model.forward(x)
```

Correct!

Silent error. Don't do it!

Here's the implementation of `Module._call_` (we left out the bits related to the JIT and made some simplifications for clarity; torch/nn/modules/module.py, line 483, class: Module):

```
def __call__(self, *input, **kwargs):
    for hook in self._forward_pre_hooks.values():
        hook(self, input)

    result = self.forward(*input, **kwargs)

    for hook in self._forward_hooks.values():
        hook_result = hook(self, input, result)
```

```
        # ...

    for hook in self._backward_hooks.values():
        # ...

    return result
```

As we can see, there are a lot of hooks that won't get called properly if we just use `.forward(…)` directly.

6.2.2 Returning to the linear model

Back to our linear model. The constructor to `nn.Linear` accepts three arguments: the number of input features, the number of output features, and whether the linear model includes a bias or not (defaulting to `True`, here):

```
# In[5]:
import torch.nn as nn

linear_model = nn.Linear(1, 1)
linear_model(t_un_val)

# Out[5]:
tensor([[0.6018],
        [0.2877]], grad_fn=<AddmmBackward>)
```

The arguments are input size, output size, and bias defaulting to True.

The number of features in our case just refers to the size of the input and the output tensor for the module, so 1 and 1. If we used both temperature and barometric pressure as input, for instance, we would have two features in input and one feature in output. As we will see, for more complex models with several intermediate modules, the number of features will be associated with the capacity of the model.

We have an instance of `nn.Linear` with one input and one output feature. That only requires one weight and one bias:

```
# In[6]:
linear_model.weight

# Out[6]:
Parameter containing:
tensor([[-0.0674]], requires_grad=True)

# In[7]:
linear_model.bias

# Out[7]:
Parameter containing:
tensor([0.7488], requires_grad=True)
```

We can call the module with some input:

```
# In[8]:
x = torch.ones(1)
linear_model(x)

# Out[8]:
tensor([0.6814], grad_fn=<AddBackward0>)
```

Although PyTorch lets us get away with it, we don't actually provide an input with the right dimensionality. We have a model that takes one input and produces one output, but PyTorch `nn.Module` and its subclasses are designed to do so on multiple samples at the same time. To accommodate multiple samples, modules expect the zeroth dimension of the input to be the number of samples in the *batch*. We encountered this concept in chapter 4, when we learned how to arrange real-world data into tensors.

BATCHING INPUTS

Any module in `nn` is written to produce outputs for a *batch* of multiple inputs at the same time. Thus, assuming we need to run `nn.Linear` on 10 samples, we can create an input tensor of size $B \times Nin$, where B is the size of the batch and Nin is the number of input features, and run it once through the model. For example:

```
# In[9]:
x = torch.ones(10, 1)
linear_model(x)

# Out[9]:
tensor([[0.6814],
        [0.6814],
        [0.6814],
        [0.6814],
        [0.6814],
        [0.6814],
        [0.6814],
        [0.6814],
        [0.6814],
        [0.6814]], grad_fn=<AddmmBackward>)
```

Let's dig into what's going on here, with figure 6.7 showing a similar situation with batched image data. Our input is $B \times C \times H \times W$ with a batch size of 3 (say, images of a dog, a bird, and then a car), three channel dimensions (red, green, and blue), and an unspecified number of pixels for height and width. As we can see, the output is a tensor of size $B \times Nout$, where $Nout$ is the number of output features: four, in this case.

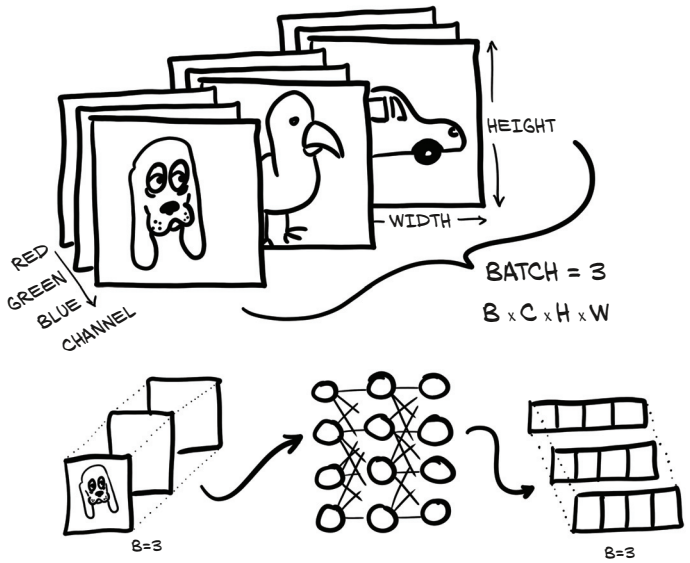


Figure 6.7 Three RGB images batched together and fed into a neural network. The output is a batch of three vectors of size 4.

Optimizing batches

The reason we want to do this batching is multifaceted. One big motivation is to make sure the computation we're asking for is big enough to saturate the computing resources we're using to perform the computation. GPUs in particular are highly parallelized, so a single input on a small model will leave most of the computing units idle. By providing batches of inputs, the calculation can be spread across the otherwise-idle units, which means the batched results come back just as quickly as a single result would. Another benefit is that some advanced models use statistical information from the entire batch, and those statistics get better with larger batch sizes.

Back to our thermometer data, `t_u` and `t_c` were two 1D tensors of size `B`. Thanks to broadcasting, we could write our linear model as `w * x + b`, where `w` and `b` were two scalar parameters. This worked because we had a single input feature: if we had two, we would need to add an extra dimension to turn that 1D tensor into a matrix with samples in the rows and features in the columns.

That's exactly what we need to do to switch to using `nn.Linear`. We reshape our *B* inputs to $B \times Nin$, where *Nin* is 1. That is easily done with `unsqueeze`:

```
# In[2]:
t_c = [0.5,  14.0, 15.0, 28.0, 11.0,  8.0,  3.0, -4.0,  6.0, 13.0, 21.0]
t_u = [35.7, 55.9, 58.2, 81.9, 56.3, 48.9, 33.9, 21.8, 48.4, 60.4, 68.4]
t_c = torch.tensor(t_c).unsqueeze(1)
t_u = torch.tensor(t_u).unsqueeze(1)

t_u.shape

# Out[2]:
torch.Size([11, 1])
```

Adds the extra dimension at axis 1

We're done; let's update our training code. First, we replace our handmade model with `nn.Linear(1,1)`, and then we need to pass the linear model parameters to the optimizer:

```
# In[10]:
linear_model = nn.Linear(1, 1)
optimizer = optim.SGD(
    linear_model.parameters(),
    lr=1e-2)
```

This is just a redefinition from earlier.

This method call replaces [params].

Earlier, it was our responsibility to create parameters and pass them as the first argument to `optim.SGD`. Now we can use the `parameters` method to ask any `nn.Module` for a list of parameters owned by it or any of its submodules:

```
# In[11]:
linear_model.parameters()

# Out[11]:
<generator object Module.parameters at 0x7f94b4a8a750>

# In[12]:
list(linear_model.parameters())

# Out[12]:
[Parameter containing:
 tensor([[0.7398]], requires_grad=True), Parameter containing:
 tensor([0.7974], requires_grad=True)]
```

This call recurses into submodules defined in the module's `init` constructor and returns a flat list of all parameters encountered, so that we can conveniently pass it to the optimizer constructor as we did previously.

We can already figure out what happens in the training loop. The optimizer is provided with a list of tensors that were defined with `requires_grad = True`—all `Parameters` are defined this way by definition, since they need to be optimized by gradient descent. When `training_loss.backward()` is called, `grad` is accumulated on the leaf nodes of the graph, which are precisely the parameters that were passed to the optimizer.

At this point, the SGD optimizer has everything it needs. When `optimizer.step()` is called, it will iterate through each `Parameter` and change it by an amount proportional to what is stored in its `grad` attribute. Pretty clean design.

Let's take a look a the training loop now:

```
# In[13]:
def training_loop(n_epochs, optimizer, model, loss_fn, t_u_train, t_u_val,
                  t_c_train, t_c_val):
    for epoch in range(1, n_epochs + 1):
        t_p_train = model(t_u_train)
        loss_train = loss_fn(t_p_train, t_c_train)

        t_p_val = model(t_u_val)
```

The model is now passed in, instead of the individual params.

```
        loss_val = loss_fn(t_p_val, t_c_val)

        optimizer.zero_grad()
        loss_train.backward()
        optimizer.step()

        if epoch == 1 or epoch % 1000 == 0:
            print(f"Epoch {epoch}, Training loss {loss_train.item():.4f},"
                  f" Validation loss {loss_val.item():.4f}")
```

The loss function is also passed in. We'll use it in a moment.

It hasn't changed practically at all, except that now we don't pass `params` explicitly to `model` since the model itself holds its `Parameters` internally.

There's one last bit that we can leverage from `torch.nn`: the loss. Indeed, `nn` comes with several common loss functions, among them `nn.MSELoss` (MSE stands for Mean Square Error), which is exactly what we defined earlier as our `loss_fn`. Loss functions in `nn` are still subclasses of `nn.Module`, so we will create an instance and call it as a function. In our case, we get rid of the handwritten `loss_fn` and replace it:

```
# In[15]:
linear_model = nn.Linear(1, 1)
optimizer = optim.SGD(linear_model.parameters(), lr=1e-2)

training_loop(
    n_epochs = 3000,
    optimizer = optimizer,
    model = linear_model,
    loss_fn = nn.MSELoss(),
    t_u_train = t_un_train,
    t_u_val = t_un_val,
    t_c_train = t_c_train,
    t_c_val = t_c_val)

print()
print(linear_model.weight)
print(linear_model.bias)

# Out[15]:
Epoch 1, Training loss 134.9599, Validation loss 183.1707
Epoch 1000, Training loss 4.8053, Validation loss 4.7307
Epoch 2000, Training loss 3.0285, Validation loss 3.0889
Epoch 3000, Training loss 2.8569, Validation loss 3.9105

Parameter containing:
tensor([[5.4319]], requires_grad=True)
Parameter containing:
tensor([-17.9693], requires_grad=True)
```

We are no longer using our hand-written loss function from earlier.

Everything else input into our training loop stays the same. Even our results remain the same as before. Of course, getting the same results is expected, as a difference would imply a bug in one of the two implementations.

6.3 Finally a neural network

It's been a long journey—there has been a lot to explore for these 20-something lines of code we require to define and train a model. Hopefully by now the magic involved in training has vanished and left room for the mechanics. What we learned so far will allow us to own the code we write instead of merely poking at a black box when things get more complicated.

There's one last step left to take: replacing our linear model with a neural network as our approximating function. We said earlier that using a neural network will not result in a higher-quality model, since the process underlying our calibration problem was fundamentally linear. However, it's good to make the leap from linear to neural network in a controlled environment so we won't feel lost later.

6.3.1 Replacing the linear model

We are going to keep everything else fixed, including the loss function, and only redefine `model`. Let's build the simplest possible neural network: a linear module, followed by an activation function, feeding into another linear module. The first linear + activation layer is commonly referred to as a *hidden* layer for historical reasons, since its outputs are not observed directly but fed into the output layer. While the input and output of the model are both of size 1 (they have one input and one output feature), the size of the output of the first linear module is usually larger than 1. Recalling our earlier explanation of the role of activations, this can lead different units to respond to different ranges of the input, which increases the capacity of our model. The last linear layer will take the output of activations and combine them linearly to produce the output value.

There is no standard way to depict neural networks. Figure 6.8 shows two ways that seem to be somewhat prototypical: the left side shows how our network might be depicted in basic introductions, whereas a style similar to that on the right is often used in the more advanced literature and research papers. It is common to make diagram blocks that roughly correspond to the neural network modules PyTorch offers (though sometimes things like the `Tanh` activation layer are not explicitly shown). Note that one somewhat subtle difference between the two is that the graph on the left has the inputs and (intermediate) results in the circles as the main elements. On the right, the computational steps are more prominent.

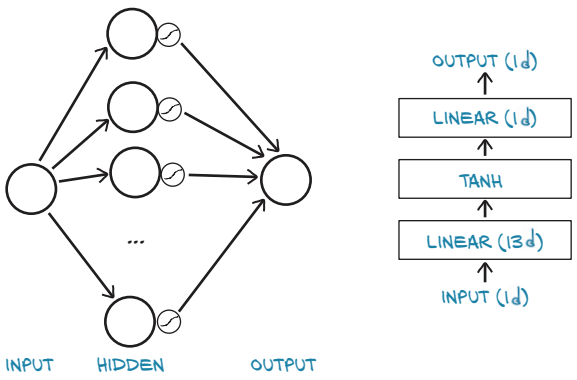


Figure 6.8 Our simplest neural network in two views. Left: beginner's version. Right: higher-level version.

`nn` provides a simple way to concatenate modules through the `nn.Sequential` container:

```
# In[16]:
seq_model = nn.Sequential(
            nn.Linear(1, 13),
            nn.Tanh(),
            nn.Linear(13, 1))
seq_model
```

We chose 13 arbitrarily. We wanted a number that was a different size from the other tensor shapes we have floating around.

This 13 must match the first size, however.

```
# Out[16]:
Sequential(
  (0): Linear(in_features=1, out_features=13, bias=True)
  (1): Tanh()
  (2): Linear(in_features=13, out_features=1, bias=True)
)
```

The end result is a model that takes the inputs expected by the first module specified as an argument of `nn.Sequential`, passes intermediate outputs to subsequent modules, and produces the output returned by the last module. The model fans out from 1 input feature to 13 hidden features, passes them through a `tanh` activation, and linearly combines the resulting 13 numbers into 1 output feature.

6.3.2 Inspecting the parameters

Calling `model.parameters()` will collect `weight` and `bias` from both the first and second linear modules. It's instructive to inspect the parameters in this case by printing their shapes:

```
# In[17]:
[param.shape for param in seq_model.parameters()]

# Out[17]:
[torch.Size([13, 1]), torch.Size([13]), torch.Size([1, 13]), torch.Size([1])]
```

These are the tensors that the optimizer will get. Again, after we call `model.backward()`, all parameters are populated with their `grad`, and the optimizer then updates their values accordingly during the `optimizer.step()` call. Not that different from our previous linear model, eh? After all, they're both differentiable models that can be trained using gradient descent.

A few notes on parameters of `nn.Modules`. When inspecting parameters of a model made up of several submodules, it is handy to be able to identify parameters by name. There's a method for that, called `named_parameters`:

```
# In[18]:
for name, param in seq_model.named_parameters():
    print(name, param.shape)

# Out[18]:
0.weight torch.Size([13, 1])
```

```
0.bias torch.Size([13])
2.weight torch.Size([1, 13])
2.bias torch.Size([1])
```

The name of each module in `Sequential` is just the ordinal with which the module appears in the arguments. Interestingly, `Sequential` also accepts an `OrderedDict`,[4] in which we can name each module passed to `Sequential`:

```
# In[19]:
from collections import OrderedDict

seq_model = nn.Sequential(OrderedDict([
    ('hidden_linear', nn.Linear(1, 8)),
    ('hidden_activation', nn.Tanh()),
    ('output_linear', nn.Linear(8, 1))
]))

seq_model
```

```
# Out[19]:
Sequential(
  (hidden_linear): Linear(in_features=1, out_features=8, bias=True)
  (hidden_activation): Tanh()
  (output_linear): Linear(in_features=8, out_features=1, bias=True)
)
```

This allows us to get more explanatory names for submodules:

```
# In[20]:
for name, param in seq_model.named_parameters():
    print(name, param.shape)
```

```
# Out[20]:
hidden_linear.weight torch.Size([8, 1])
hidden_linear.bias torch.Size([8])
output_linear.weight torch.Size([1, 8])
output_linear.bias torch.Size([1])
```

This is more descriptive; but it does not give us more flexibility in the flow of data through the network, which remains a purely sequential pass-through—the `nn.Sequential` is very aptly named. We will see how to take full control of the processing of input data by subclassing `nn.Module` ourselves in chapter 8.

We can also access a particular `Parameter` by using submodules as attributes:

```
# In[21]:
seq_model.output_linear.bias
```

```
# Out[21]:
Parameter containing:
tensor([-0.0173], requires_grad=True)
```

[4] Not all versions of Python specify the iteration order for `dict`, so we're using `OrderedDict` here to ensure the ordering of the layers and emphasize that the order of the layers matters.

This is useful for inspecting parameters or their gradients: for instance, to monitor gradients during training, as we did at the beginning of this chapter. Say we want to print out the gradients of `weight` of the linear portion of the hidden layer. We can run the training loop for the new neural network model and then look at the resulting gradients after the last epoch:

```
# In[22]:
optimizer = optim.SGD(seq_model.parameters(), lr=1e-3)

training_loop(
    n_epochs = 5000,
    optimizer = optimizer,
    model = seq_model,
    loss_fn = nn.MSELoss(),
    t_u_train = t_un_train,
    t_u_val = t_un_val,
    t_c_train = t_c_train,
    t_c_val = t_c_val)

print('output', seq_model(t_un_val))
print('answer', t_c_val)
print('hidden', seq_model.hidden_linear.weight.grad)

# Out[22]:
Epoch 1, Training loss 182.9724, Validation loss 231.8708
Epoch 1000, Training loss 6.6642, Validation loss 3.7330
Epoch 2000, Training loss 5.1502, Validation loss 0.1406
Epoch 3000, Training loss 2.9653, Validation loss 1.0005
Epoch 4000, Training loss 2.2839, Validation loss 1.6580
Epoch 5000, Training loss 2.1141, Validation loss 2.0215
output tensor([[-1.9930],
        [20.8729]], grad_fn=<AddmmBackward>)
answer tensor([[-4.],
        [21.]])
hidden tensor([[ 0.0272],
        [ 0.0139],
        [ 0.1692],
        [ 0.1735],
        [-0.1697],
        [ 0.1455],
        [-0.0136],
        [-0.0554]])
```

We've dropped the learning rate a bit to help with stability.

6.3.3 Comparing to the linear model

We can also evaluate the model on all of the data and see how it differs from a line:

```
# In[23]:
from matplotlib import pyplot as plt

t_range = torch.arange(20., 90.).unsqueeze(1)

fig = plt.figure(dpi=600)
```

```
plt.xlabel("Fahrenheit")
plt.ylabel("Celsius")
plt.plot(t_u.numpy(), t_c.numpy(), 'o')
plt.plot(t_range.numpy(), seq_model(0.1 * t_range).detach().numpy(), 'c-')
plt.plot(t_u.numpy(), seq_model(0.1 * t_u).detach().numpy(), 'kx')
```

The result is shown in figure 6.9. We can appreciate that the neural network has a tendency to overfit, as we discussed in chapter 5, since it tries to chase the measurements, including the noisy ones. Even our tiny neural network has too many parameters to fit the few measurements we have. It doesn't do a bad job, though, overall.

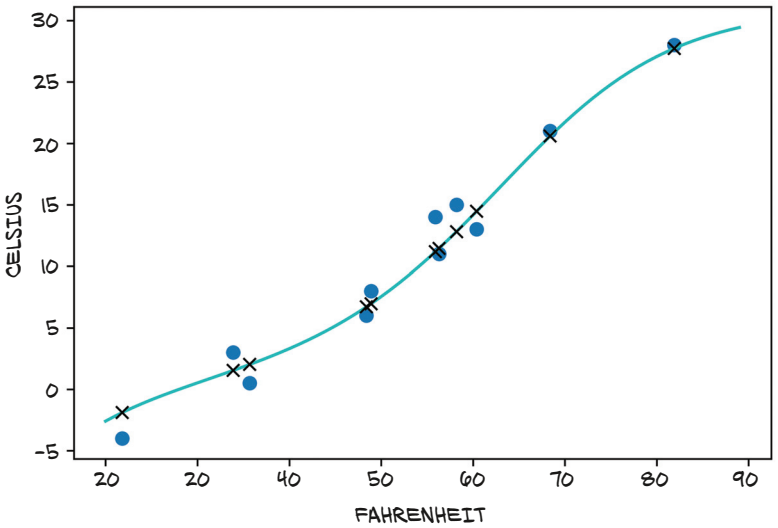


Figure 6.9 The plot of our neural network model, with input data (circles) and model output (Xs). The continuous line shows behavior between samples.

6.4 Conclusion

We've covered a lot in chapters 5 and 6, although we have been dealing with a very simple problem. We dissected building differentiable models and training them using gradient descent, first using raw autograd and then relying on `nn`. By now you should have confidence in your understanding of what's going on behind the scenes. Hopefully this taste of PyTorch has given you an appetite for more!

6.5 Exercises

1. Experiment with the number of hidden neurons in our simple neural network model, as well as the learning rate.
   a. What changes result in more linear output from the model?
   b. Can you get the model to obviously overfit the data?

2. The third-hardest problem in physics is finding a proper wine to celebrate discoveries. Load the wine data from chapter 4, and create a new model with the appropriate number of input parameters.
   a. How long does it take to train compared to the temperature data we have been using?
   b. Can you explain what factors contribute to the training times?
   c. Can you get the loss to decrease while training on this dataset?
   d. How would you go about graphing this dataset?

6.6 Summary

- Neural networks can be automatically adapted to specialize themselves on the problem at hand.
- Neural networks allow easy access to the analytical derivatives of the loss with respect to any parameter in the model, which makes evolving the parameters very efficient. Thanks to its automated differentiation engine, PyTorch provides such derivatives effortlessly.
- Activation functions around linear transformations make neural networks capable of approximating highly nonlinear functions, at the same time keeping them simple enough to optimize.
- The `nn` module together with the tensor standard library provide all the building blocks for creating neural networks.
- To recognize overfitting, it's essential to maintain the training set of data points separate from the validation set. There's no one recipe to combat overfitting, but getting more data, or more variability in the data, and resorting to simpler models are good starts.
- Anyone doing data science should be plotting data all the time.

7 Telling birds from airplanes: Learning from images

This chapter covers

- Building a feed-forward neural network
- Loading data using `Dataset`s and `DataLoader`s
- Understanding classification loss

The last chapter gave us the opportunity to dive into the inner mechanics of learning through gradient descent, and the facilities that PyTorch offers to build models and optimize them. We did so using a simple regression model of one input and one output, which allowed us to have everything in plain sight but admittedly was only borderline exciting.

In this chapter, we'll keep moving ahead with building our neural network foundations. This time, we'll turn our attention to images. Image recognition is arguably the task that made the world realize the potential of deep learning.

We will approach a simple image recognition problem step by step, building from a simple neural network like the one we defined in the last chapter. This time, instead of a tiny dataset of numbers, we'll use a more extensive dataset of tiny images. Let's download the dataset first and get to work preparing it for use.

7.1 A dataset of tiny images

There is nothing like an intuitive understanding of a subject, and there is nothing to achieve that like working on simple data. One of the most basic datasets for image recognition is the handwritten digit-recognition dataset known as MNIST. Here we will use another dataset that is similarly simple and a bit more fun. It's called CIFAR-10, and, like its sibling CIFAR-100, it has been a computer vision classic for a decade.

CIFAR-10 consists of 60,000 tiny 32 × 32 color (RGB) images, labeled with an integer corresponding to 1 of 10 classes: airplane (0), automobile (1), bird (2), cat (3), deer (4), dog (5), frog (6), horse (7), ship (8), and truck (9).[1] Nowadays, CIFAR-10 is considered too simple for developing or validating new research, but it serves our learning purposes just fine. We will use the `torchvision` module to automatically download the dataset and load it as a collection of PyTorch tensors. Figure 7.1 gives us a taste of CIFAR-10.

Figure 7.1 Image samples from all CIFAR-10 classes

[1] The images were collected and labeled by Krizhevsky, Nair, and Hinton of the Canadian Institute For Advanced Research (CIFAR) and were drawn from a larger collection of unlabeled 32 × 32 color images: the "80 million tiny images dataset" from the Computer Science and Artificial Intelligence Laboratory (CSAIL) at the Massachusetts Institute of Technology.

7.1.1 Downloading CIFAR-10

As we anticipated, let's import `torchvision` and use the `datasets` module to download the CIFAR-10 data:

Instantiates a dataset for the training data; TorchVision downloads the data if it is not present.

With train=False, this gets us a dataset for the validation data, again downloading as necessary.

```
# In[2]:
from torchvision import datasets
data_path = '../data-unversioned/p1ch7/'
cifar10 = datasets.CIFAR10(data_path, train=True, download=True)
cifar10_val = datasets.CIFAR10(data_path, train=False, download=True)
```

The first argument we provide to the `CIFAR10` function is the location from which the data will be downloaded; the second specifies whether we're interested in the training set or the validation set; and the third says whether we allow PyTorch to download the data if it is not found in the location specified in the first argument.

Just like `CIFAR10`, the `datasets` submodule gives us precanned access to the most popular computer vision datasets, such as MNIST, Fashion-MNIST, CIFAR-100, SVHN, Coco, and Omniglot. In each case, the dataset is returned as a subclass of `torch.utils.data.Dataset`. We can see that the method-resolution order of our `cifar10` instance includes it as a base class:

```
# In[4]:
type(cifar10).__mro__
```

```
# Out[4]:
(torchvision.datasets.cifar.CIFAR10,
 torchvision.datasets.vision.VisionDataset,
 torch.utils.data.dataset.Dataset,
 object)
```

7.1.2 The Dataset class

It's a good time to discover what being a subclass of `torch.utils.data.Dataset` means in practice. Looking at figure 7.2, we see what PyTorch `Dataset` is all about. It is an object that is required to implement two methods: `__len__` and `__getitem__`. The former should return the number of items in the dataset; the latter should return the item, consisting of a sample and its corresponding label (an integer index).[2]

In practice, when a Python object is equipped with the `__len__` method, we can pass it as an argument to the `len` Python built-in function:

```
# In[5]:
len(cifar10)
```

```
# Out[5]:
50000
```

[2] For some advanced uses, PyTorch also provides `IterableDataset`. This can be used in cases like datasets in which random access to the data is prohibitively expensive or does not make sense: for example, because data is generated on the fly.

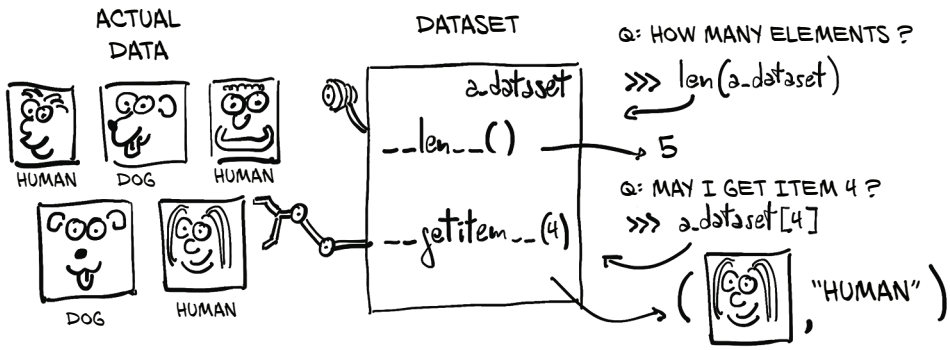


Figure 7.2 Concept of a PyTorch `Dataset` object: it doesn't necessarily hold the data, but it provides uniform access to it through `__len__` and `__getitem__`.

Similarly, since the dataset is equipped with the `__getitem__` method, we can use the standard subscript for indexing tuples and lists to access individual items. Here, we get a `PIL` (Python Imaging Library, the `PIL` package) image with our desired output—an integer with the value `1`, corresponding to "automobile":

```
# In[6]:
img, label = cifar10[99]
img, label, class_names[label]

# Out[6]:
(<PIL.Image.Image image mode=RGB size=32x32 at 0x7FB383657390>,
 1,
 'automobile')
```

So, the sample in the `data.CIFAR10` dataset is an instance of an RGB PIL image. We can plot it right away:

```
# In[7]:
plt.imshow(img)
plt.show()
```

This produces the output shown in figure 7.3. It's a red car![3]

[3] It doesn't translate well to print; you'll have to take our word for it, or check it out in the eBook or the Jupyter Notebook.

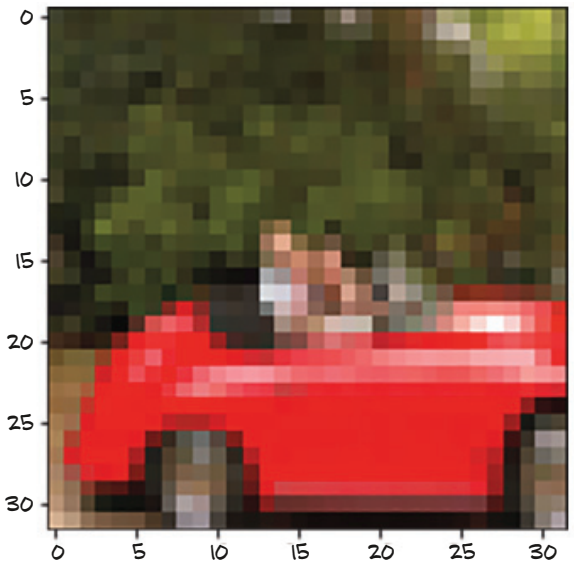


Figure 7.3 The 99th image from the CIFAR-10 dataset: an automobile

7.1.3 Dataset transforms

That's all very nice, but we'll likely need a way to convert the PIL image to a PyTorch tensor before we can do anything with it. That's where `torchvision.transforms` comes in. This module defines a set of composable, function-like objects that can be passed as an argument to a `torchvision` dataset such as `datasets.CIFAR10(…)`, and that perform transformations on the data after it is loaded but before it is returned by `__getitem__`. We can see the list of available objects as follows:

```
# In[8]:
from torchvision import transforms
dir(transforms)

# Out[8]:
['CenterCrop',
 'ColorJitter',
 ...
 'Normalize',
 'Pad',
 'RandomAffine',
 ...
 'RandomResizedCrop',
 'RandomRotation',
 'RandomSizedCrop',
 ...
 'TenCrop',
 'ToPILImage',
 'ToTensor',
 ...
]
```

Among those transforms, we can spot `ToTensor`, which turns NumPy arrays and PIL images to tensors. It also takes care to lay out the dimensions of the output tensor as $C \times H \times W$ (channel, height, width; just as we covered in chapter 4).

Let's try out the `ToTensor` transform. Once instantiated, it can be called like a function with the PIL image as the argument, returning a tensor as output:

```
# In[9]:
from torchvision import transforms

to_tensor = transforms.ToTensor()
img_t = to_tensor(img)
img_t.shape

# Out[9]:
torch.Size([3, 32, 32])
```

The image has been turned into a $3 \times 32 \times 32$ tensor and therefore a 3-channel (RGB) 32×32 image. Note that nothing has happened to `label`; it is still an integer.

As we anticipated, we can pass the transform directly as an argument to `dataset.CIFAR10`:

```
# In[10]:
tensor_cifar10 = datasets.CIFAR10(data_path, train=True, download=False,
                                  transform=transforms.ToTensor())
```

At this point, accessing an element of the dataset will return a tensor, rather than a PIL image:

```
# In[11]:
img_t, _ = tensor_cifar10[99]
type(img_t)

# Out[11]:
torch.Tensor
```

As expected, the shape has the channel as the first dimension, while the scalar type is `float32`:

```
# In[12]:
img_t.shape, img_t.dtype

# Out[12]:
(torch.Size([3, 32, 32]), torch.float32)
```

Whereas the values in the original PIL image ranged from 0 to 255 (8 bits per channel), the `ToTensor` transform turns the data into a 32-bit floating-point per channel, scaling the values down from 0.0 to 1.0. Let's verify that:

```
# In[13]:
img_t.min(), img_t.max()

# Out[13]:
(tensor(0.), tensor(1.))
```

And let's verify that we're getting the same image out:

```
# In[14]:
plt.imshow(img_t.permute(1, 2, 0))
plt.show()

# Out[14]:
<Figure size 432x288 with 1 Axes>
```

Changes the order of the axes from C × H × W to H × W × C

As we can see in figure 7.4, we get the same output as before.

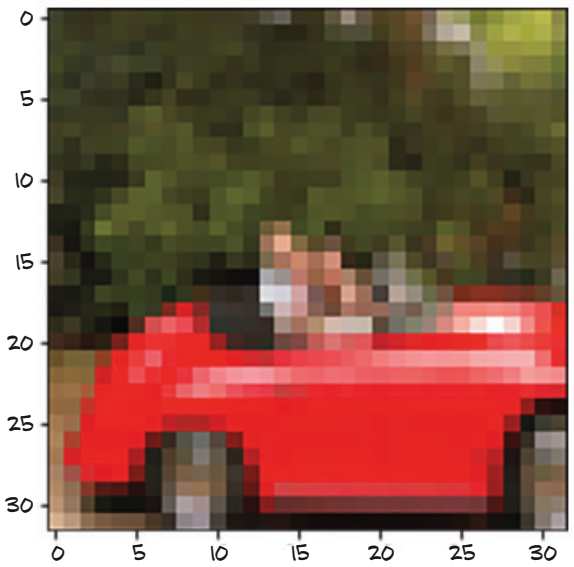


Figure 7.4 We've seen this one already.

It checks. Note how we have to use `permute` to change the order of the axes from C × H × W to H × W × C to match what Matplotlib expects.

7.1.4 Normalizing data

Transforms are really handy because we can chain them using `transforms.Compose`, and they can handle normalization and data augmentation transparently, directly in the data loader. For instance, it's good practice to normalize the dataset so that each channel has zero mean and unitary standard deviation. We mentioned this in chapter 4, but now, after going through chapter 5, we also have an intuition for why: by choosing activation functions that are linear around 0 plus or minus 1 (or 2), keeping the data in the same range means it's more likely that neurons have nonzero gradients and,

hence, will learn sooner. Also, normalizing each channel so that it has the same distribution will ensure that channel information can be mixed and updated through gradient descent using the same learning rate. This is just like the situation in section 5.4.4 when we rescaled the weight to be of the same magnitude as the bias in our temperature-conversion model.

In order to make it so that each channel has zero mean and unitary standard deviation, we can compute the mean value and the standard deviation of each channel across the dataset and apply the following transform: `v_n[c] = (v[c] - mean[c]) / stdev[c]`. This is what `transforms.Normalize` does. The values of `mean` and `stdev` must be computed offline (they are not computed by the transform). Let's compute them for the CIFAR-10 training set.

Since the CIFAR-10 dataset is small, we'll be able to manipulate it entirely in memory. Let's stack all the tensors returned by the dataset along an extra dimension:

```
# In[15]:
imgs = torch.stack([img_t for img_t, _ in tensor_cifar10], dim=3)
imgs.shape

# Out[15]:
torch.Size([3, 32, 32, 50000])
```

Now we can easily compute the mean per channel:

```
# In[16]:
imgs.view(3, -1).mean(dim=1)

# Out[16]:
tensor([0.4915, 0.4823, 0.4468])
```

Recall that view(3, -1) keeps the three channels and merges all the remaining dimensions into one, figuring out the appropriate size. Here our 3 × 32 × 32 image is transformed into a 3 × 1,024 vector, and then the mean is taken over the 1,024 elements of each channel.

Computing the standard deviation is similar:

```
# In[17]:
imgs.view(3, -1).std(dim=1)

# Out[17]:
tensor([0.2470, 0.2435, 0.2616])
```

With these numbers in our hands, we can initialize the `Normalize` transform

```
# In[18]:
transforms.Normalize((0.4915, 0.4823, 0.4468), (0.2470, 0.2435, 0.2616))

# Out[18]:
Normalize(mean=(0.4915, 0.4823, 0.4468), std=(0.247, 0.2435, 0.2616))
```

and concatenate it after the `ToTensor` transform:

```
# In[19]:
transformed_cifar10 = datasets.CIFAR10(
    data_path, train=True, download=False,
```

```
    transform=transforms.Compose([
        transforms.ToTensor(),
        transforms.Normalize((0.4915, 0.4823, 0.4468),
                             (0.2470, 0.2435, 0.2616))
    ]))
```

Note that, at this point, plotting an image drawn from the dataset won't provide us with a faithful representation of the actual image:

```
# In[21]:
img_t, _ = transformed_cifar10[99]

plt.imshow(img_t.permute(1, 2, 0))
plt.show()
```

The renormalized red car we get is shown in figure 7.5. This is because normalization has shifted the RGB levels outside the 0.0 to 1.0 range and changed the overall magnitudes of the channels. All of the data is still there; it's just that Matplotlib renders it as black. We'll keep this in mind for the future.

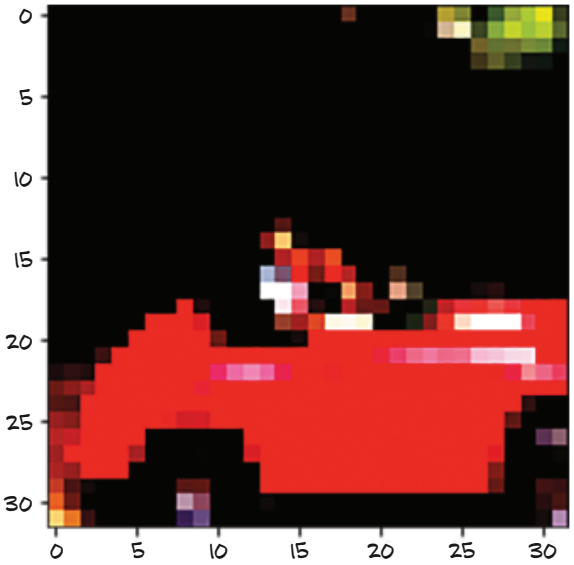


Figure 7.5 Our random CIFAR-10 image after normalization

Still, we have a fancy dataset loaded that contains tens of thousands of images! That's quite convenient, because we were going to need something exactly like it.

7.2 Distinguishing birds from airplanes

Jane, our friend at the bird-watching club, has set up a fleet of cameras in the woods south of the airport. The cameras are supposed to save a shot when something enters the frame and upload it to the club's real-time bird-watching blog. The problem is that a lot of planes coming and going from the airport end up triggering the camera,

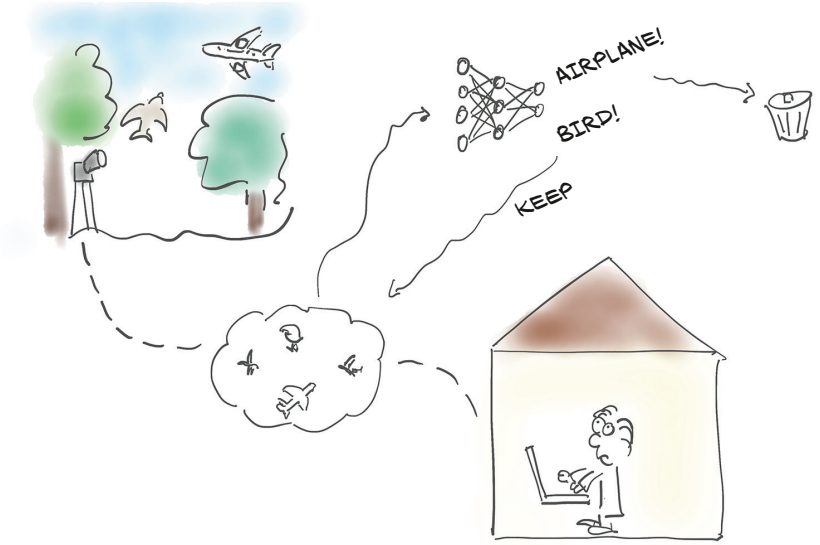


Figure 7.6 The problem at hand: we're going to help our friend tell birds from airplanes for her blog, by training a neural network to do the job.

so Jane spends a lot of time deleting pictures of airplanes from the blog. What she needs is an automated system like that shown in figure 7.6. Instead of manually deleting, she needs a neural network—an AI if we're into fancy marketing speak—to throw away the airplanes right away.

No worries! We'll take care of that, no problem—we just got the perfect dataset for it (what a coincidence, right?). We'll pick out all the birds and airplanes from our CIFAR-10 dataset and build a neural network that can tell birds and airplanes apart.

7.2.1 Building the dataset

The first step is to get the data in the right shape. We could create a `Dataset` subclass that only includes birds and airplanes. However, the dataset is small, and we only need indexing and `len` to work on our dataset. It doesn't actually have to be a subclass of `torch.utils.data.dataset.Dataset`! Well, why not take a shortcut and just filter the data in `cifar10` and remap the labels so they are contiguous? Here's how:

```
# In[5]:
label_map = {0: 0, 2: 1}
class_names = ['airplane', 'bird']
cifar2 = [(img, label_map[label])
          for img, label in cifar10
          if label in [0, 2]]
cifar2_val = [(img, label_map[label])
              for img, label in cifar10_val
              if label in [0, 2]]
```

The `cifar2` object satisfies the basic requirements for a `Dataset`—that is, `__len__` and `__getitem__` are defined—so we're going to use that. We should be aware, however, that this is a clever shortcut and we might wish to implement a proper `Dataset` if we hit limitations with it.[4]

We have a dataset! Next, we need a model to feed our data to.

7.2.2 A fully connected model

We learned how to build a neural network in chapter 5. We know that it's a tensor of features in, a tensor of features out. After all, an image is just a set of numbers laid out in a spatial configuration. OK, we don't know how to handle the spatial configuration part just yet, but in theory if we just take the image pixels and straighten them into a long 1D vector, we could consider those numbers as input features, right? This is what figure 7.7 illustrates.

Let's try that. How many features per sample? Well, $32 \times 32 \times 3$: that is, 3,072 input features per sample. Starting from the model we built in chapter 5, our new model would be an `nn.Linear` with 3,072 input features and some number of hidden features,

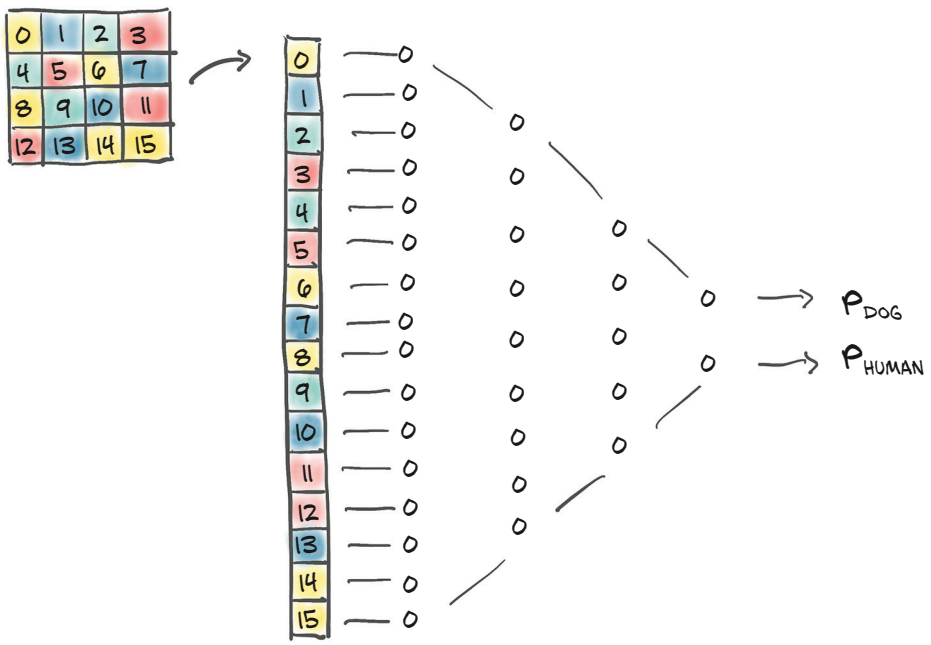


Figure 7.7 Treating our image as a 1D vector of values and training a fully connected classifier on it

[4] Here, we built the new dataset manually and also wanted to remap the classes. In some cases, it may be enough to take a subset of the indices of a given dataset. This can be accomplished using the `torch.utils.data.Subset` class. Similarly, there is `ConcatDataset` to join datasets (of compatible items) into a larger one. For iterable datasets, `ChainDataset` gives a larger, iterable dataset.

followed by an activation, and then another `nn.Linear` that tapers the network down to an appropriate output number of features (2, for this use case):

```
# In[6]:
import torch.nn as nn

n_out = 2

model = nn.Sequential(
            nn.Linear(
                3072,
                512,
            ),
            nn.Tanh(),
            nn.Linear(
                512,
                n_out,
            )
        )
```

Input features → `3072,`

Hidden layer size → `512,` (and `512,`)

Output classes → `n_out,`

We somewhat arbitrarily pick 512 hidden features. A neural network needs at least one hidden layer (of activations, so two modules) with a nonlinearity in between in order to be able to learn arbitrary functions in the way we discussed in section 6.3—otherwise, it would just be a linear model. The hidden features represent (learned) relations between the inputs encoded through the weight matrix. As such, the model might learn to "compare" vector elements 176 and 208, but it does not a priori focus on them because it is structurally unaware that these are, indeed (row 5, pixel 16) and (row 6, pixel 16), and thus adjacent.

So we have a model. Next we'll discuss what our model output should be.

7.2.3 Output of a classifier

In chapter 6, the network produced the predicted temperature (a number with a quantitative meaning) as output. We could do something similar here: make our network output a single scalar value (so `n_out = 1`), cast the labels to floats (0.0 for airplane and 1.0 for bird), and use those as a target for `MSELoss` (the average of squared differences in the batch). Doing so, we would cast the problem into a regression problem. However, looking more closely, we are now dealing with something a bit different in nature.[5]

We need to recognize that the output is categorical: it's either a bird or an airplane (or something else if we had all 10 of the original classes). As we learned in chapter 4, when we have to represent a categorical variable, we should switch to a one-hot-encoding representation of that variable, such as `[1, 0]` for airplane or `[0, 1]`

[5] Using distance on the "probability" vectors would already have been much better than using `MSELoss` with the class numbers—which, recalling our discussion of types of values in the sidebar "Continuous, ordinal, and categorical values" from chapter 4, does not make sense for categories and does not work at all in practice. Still, `MSELoss` is not very well suited to classification problems.

for bird (the order is arbitrary). This will still work if we have 10 classes, as in the full CIFAR-10 dataset; we'll just have a vector of length 10.[6]

In the ideal case, the network would output `torch.tensor([1.0, 0.0])` for an airplane and `torch.tensor([0.0, 1.0])` for a bird. Practically speaking, since our classifier will not be perfect, we can expect the network to output something in between. The key realization in this case is that we can interpret our output as probabilities: the first entry is the probability of "airplane," and the second is the probability of "bird."

Casting the problem in terms of probabilities imposes a few extra constraints on the outputs of our network:

- Each element of the output must be in the `[0.0, 1.0]` range (a probability of an outcome cannot be less than 0 or greater than 1).
- The elements of the output must add up to 1.0 (we're certain that one of the two outcomes will occur).

It sounds like a tough constraint to enforce in a differentiable way on a vector of numbers. Yet there's a very smart trick that does exactly that, and it's differentiable: it's called *softmax*.

7.2.4 Representing the output as probabilities

Softmax is a function that takes a vector of values and produces another vector of the same dimension, where the values satisfy the constraints we just listed to represent probabilities. The expression for softmax is shown in figure 7.8.

That is, we take the elements of the vector, compute the elementwise exponential, and divide each element by the sum of exponentials. In code, it's something like this:

```
# In[7]:
def softmax(x):
    return torch.exp(x) / torch.exp(x).sum()
```

Let's test it on an input vector:

```
# In[8]:
x = torch.tensor([1.0, 2.0, 3.0])

softmax(x)

# Out[8]:
tensor([0.0900, 0.2447, 0.6652])
```

[6] For the special binary classification case, using two values here is redundant, as one is always 1 minus the other. And indeed PyTorch lets us output only a single probability using the `nn.Sigmoid` activation at the end of the model to get a probability and the binary cross-entropy loss function `nn.BCELoss`. There also is an `nn.BCELossWithLogits` merging these two steps.

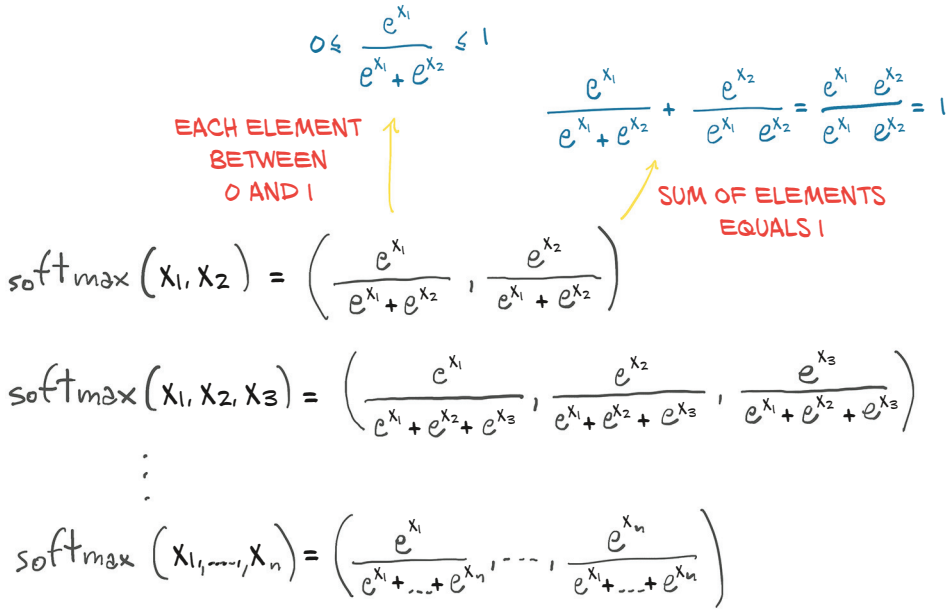


Figure 7.8 Handwritten softmax

As expected, it satisfies the constraints on probability:

```
# In[9]:
softmax(x).sum()

# Out[9]:
tensor(1.)
```

Softmax is a monotone function, in that lower values in the input will correspond to lower values in the output. However, it's not *scale invariant*, in that the ratio between values is not preserved. In fact, the ratio between the first and second elements of the input is 0.5, while the ratio between the same elements in the output is 0.3678. This is not a real issue, since the learning process will drive the parameters of the model in a way that values have appropriate ratios.

The `nn` module makes softmax available as a module. Since, as usual, input tensors may have an additional batch 0th dimension, or have dimensions along which they encode probabilities and others in which they don't, `nn.Softmax` requires us to specify the dimension along which the softmax function is applied:

```
# In[10]:
softmax = nn.Softmax(dim=1)

x = torch.tensor([[1.0, 2.0, 3.0],
                  [1.0, 2.0, 3.0]])
```

```
softmax(x)

# Out[10]:
tensor([[0.0900, 0.2447, 0.6652],
        [0.0900, 0.2447, 0.6652]])
```

In this case, we have two input vectors in two rows (just like when we work with batches), so we initialize `nn.Softmax` to operate along dimension 1.

Excellent! We can now add a softmax at the end of our model, and our network will be equipped to produce probabilities:

```
# In[11]:
model = nn.Sequential(
            nn.Linear(3072, 512),
            nn.Tanh(),
            nn.Linear(512, 2),
            nn.Softmax(dim=1))
```

We can actually try running the model before even training it. Let's do it, just to see what comes out. We first build a batch of one image, our bird (figure 7.9):

```
# In[12]:
img, _ = cifar2[0]

plt.imshow(img.permute(1, 2, 0))
plt.show()
```

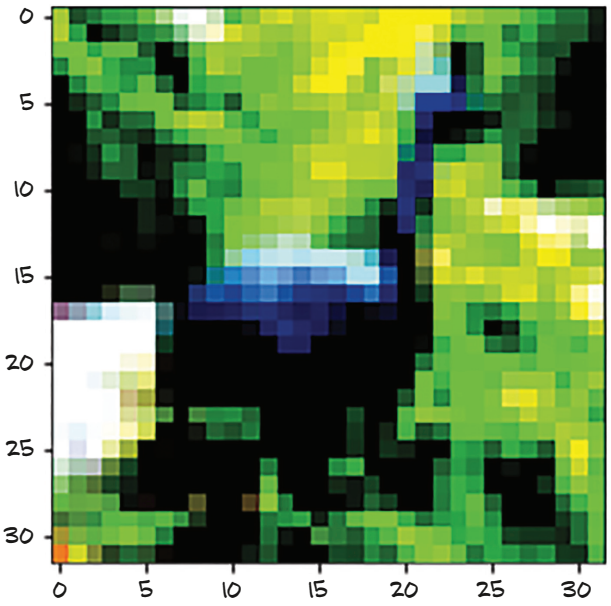


Figure 7.9 A random bird from the CIFAR-10 dataset (after normalization)

Oh, hello there. In order to call the model, we need to make the input have the right dimensions. We recall that our model expects 3,072 features in the input, and that `nn` works with data organized into batches along the zeroth dimension. So we need to turn our 3 × 32 × 32 image into a 1D tensor and then add an extra dimension in the zeroth position. We learned how to do this in chapter 3:

```
# In[13]:
img_batch = img.view(-1).unsqueeze(0)
```

Now we're ready to invoke our model:

```
# In[14]:
out = model(img_batch)
out

# Out[14]:
tensor([[0.4784, 0.5216]], grad_fn=<SoftmaxBackward>)
```

So, we got probabilities! Well, we know we shouldn't get too excited: the weights and biases of our linear layers have not been trained at all. Their elements are initialized randomly by PyTorch between –1.0 and 1.0. Interestingly, we also see `grad_fn` for the output, which is the tip of the backward computation graph (it will be used as soon as we need to backpropagate).[7]

In addition, while we know which output probability is supposed to be which (recall our `class_names`), our network has no indication of that. Is the first entry "airplane" and the second "bird," or the other way around? The network can't even tell that at this point. It's the loss function that associates a meaning with these two numbers, after backpropagation. If the labels are provided as index 0 for "airplane" and index 1 for "bird," then that's the order the outputs will be induced to take. Thus, after training, we will be able to get the label as an index by computing the *argmax* of the output probabilities: that is, the index at which we get the maximum probability. Conveniently, when supplied with a dimension, `torch.max` returns the maximum element along that dimension as well as the index at which that value occurs. In our case, we need to take the max along the probability vector (not across batches), therefore, dimension 1:

```
# In[15]:
_, index = torch.max(out, dim=1)

index

# Out[15]:
tensor([1])
```

[7] While it is, in principle, possible to say that here the model is uncertain (because it assigns 48% and 52% probabilities to the two classes), it will turn out that typical training results in highly overconfident models. Bayesian neural networks can provide some remedy, but they are beyond the scope of this book.

It says the image is a bird. Pure luck. But we have adapted our model output to the classification task at hand by getting it to output probabilities. We also have now run our model against an input image and verified that our plumbing works. Time to get training. As in the previous two chapters, we need a loss to minimize during training.

7.2.5 A loss for classifying

We just mentioned that the loss is what gives probabilities meaning. In chapters 5 and 6, we used mean square error (MSE) as our loss. We could still use MSE and make our output probabilities converge to `[0.0, 1.0]` and `[1.0, 0.0]`. However, thinking about it, we're not really interested in reproducing these values exactly. Looking back at the argmax operation we used to extract the index of the predicted class, what we're really interested in is that the first probability is higher than the second for airplanes and vice versa for birds. In other words, we want to penalize misclassifications rather than painstakingly penalize everything that doesn't look exactly like a 0.0 or 1.0.

What we need to maximize in this case is the probability associated with the correct class, `out[class_index]`, where `out` is the output of softmax and `class_index` is a vector containing 0 for "airplane" and 1 for "bird" for each sample. This quantity—that is, the probability associated with the correct class—is referred to as the *likelihood* (of our model's parameters, given the data).[8] In other words, we want a loss function that is very high when the likelihood is low: so low that the alternatives have a higher probability. Conversely, the loss should be low when the likelihood is higher than the alternatives, and we're not really fixated on driving the probability up to 1.

There's a loss function that behaves that way, and it's called *negative log likelihood* (NLL). It has the expression `NLL = - sum(log(out_i[c_i]))`, where the sum is taken over N samples and `c_i` is the correct class for sample i. Let's take a look at figure 7.10, which shows the NLL as a function of predicted probability.

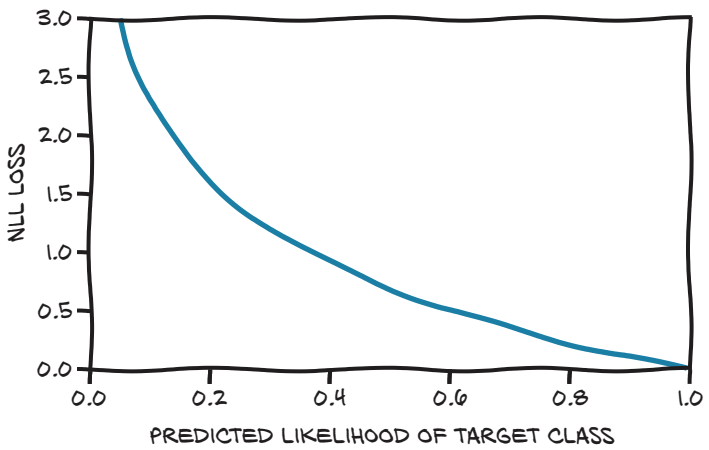


Figure 7.10 The NLL loss as a function of the predicted probabilities

[8] For a succinct definition of the terminology, refer to David MacKay's *Information Theory, Inference, and Learning Algorithms* (Cambridge University Press, 2003), section 2.3.

The figure shows that when low probabilities are assigned to the data, the NLL grows to infinity, whereas it decreases at a rather shallow rate when probabilities are greater than 0.5. Remember that the NLL takes probabilities as input; so, as the likelihood grows, the other probabilities will necessarily decrease.

Summing up, our loss for classification can be computed as follows. For each sample in the batch:

1. Run the forward pass, and obtain the output values from the last (linear) layer.
2. Compute their softmax, and obtain probabilities.
3. Take the predicted probability corresponding to the correct class (the likelihood of the parameters). Note that we know what the correct class is because it's a supervised problem—it's our ground truth.
4. Compute its logarithm, slap a minus sign in front of it, and add it to the loss.

So, how do we do this in PyTorch? PyTorch has an `nn.NLLLoss` class. However (gotcha ahead), as opposed to what you might expect, it does not take probabilities but rather takes a tensor of log probabilities as input. It then computes the NLL of our model given the batch of data. There's a good reason behind the input convention: taking the logarithm of a probability is tricky when the probability gets close to zero. The workaround is to use `nn.LogSoftmax` instead of `nn.Softmax`, which takes care to make the calculation numerically stable.

We can now modify our model to use `nn.LogSoftmax` as the output module:

```
model = nn.Sequential(
            nn.Linear(3072, 512),
            nn.Tanh(),
            nn.Linear(512, 2),
            nn.LogSoftmax(dim=1))
```

Then we instantiate our NLL loss:

```
loss = nn.NLLLoss()
```

The loss takes the output of `nn.LogSoftmax` for a batch as the first argument and a tensor of class indices (zeros and ones, in our case) as the second argument. We can now test it with our birdie:

```
img, label = cifar2[0]

out = model(img.view(-1).unsqueeze(0))

loss(out, torch.tensor([label]))

tensor(0.6509, grad_fn=<NllLossBackward>)
```

Ending our investigation of losses, we can look at how using cross-entropy loss improves over MSE. In figure 7.11, we see that the cross-entropy loss has some slope

when the prediction is off target (in the low-loss corner, the correct class is assigned a predicted probability of 99.97%), while the MSE we dismissed at the beginning saturates much earlier and—crucially—also for very wrong predictions. The underlying reason is that the slope of the MSE is too low to compensate for the flatness of the softmax function for wrong predictions. This is why the MSE for probabilities is not a good fit for classification work.

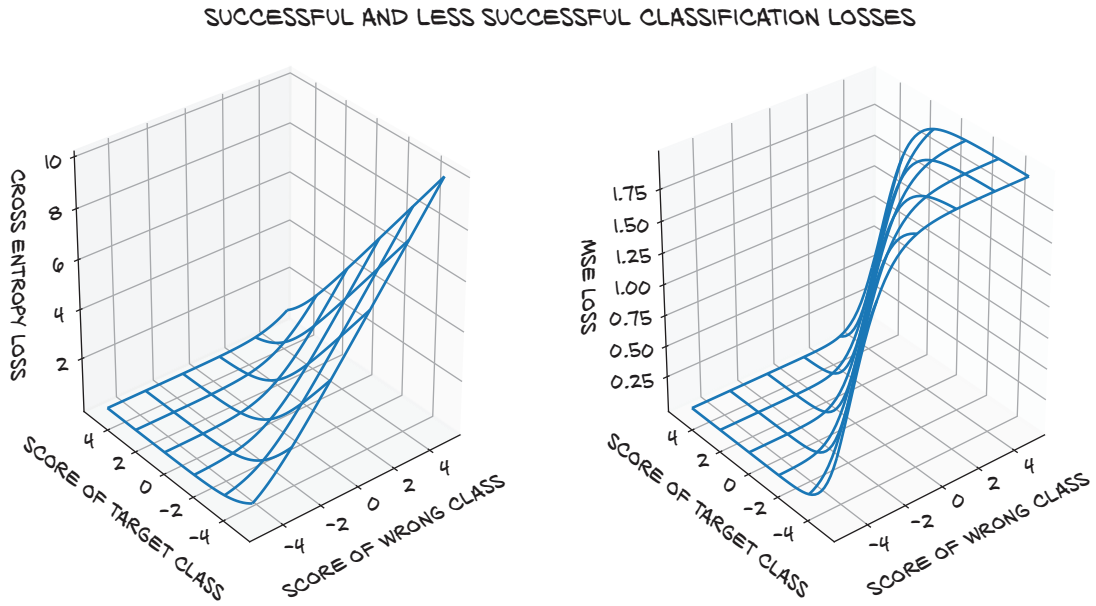


Figure 7.11 The cross entropy (left) and MSE between predicted probabilities and the target probability vector (right) as functions of the predicted scores—that is, before the (log-) softmax

7.2.6 Training the classifier

All right! We're ready to bring back the training loop we wrote in chapter 5 and see how it trains (the process is illustrated in figure 7.12):

```
import torch
import torch.nn as nn

model = nn.Sequential(
            nn.Linear(3072, 512),
            nn.Tanh(),
            nn.Linear(512, 2),
            nn.LogSoftmax(dim=1))

learning_rate = 1e-2

optimizer = optim.SGD(model.parameters(), lr=learning_rate)
```

```
loss_fn = nn.NLLLoss()

n_epochs = 100

for epoch in range(n_epochs):
    for img, label in cifar2:
        out = model(img.view(-1).unsqueeze(0))
        loss = loss_fn(out, torch.tensor([label]))

        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

    print("Epoch: %d, Loss: %f" % (epoch, float(loss)))
```

Prints the loss for the last image. In the next chapter, we will improve our output to give an average over the entire epoch.

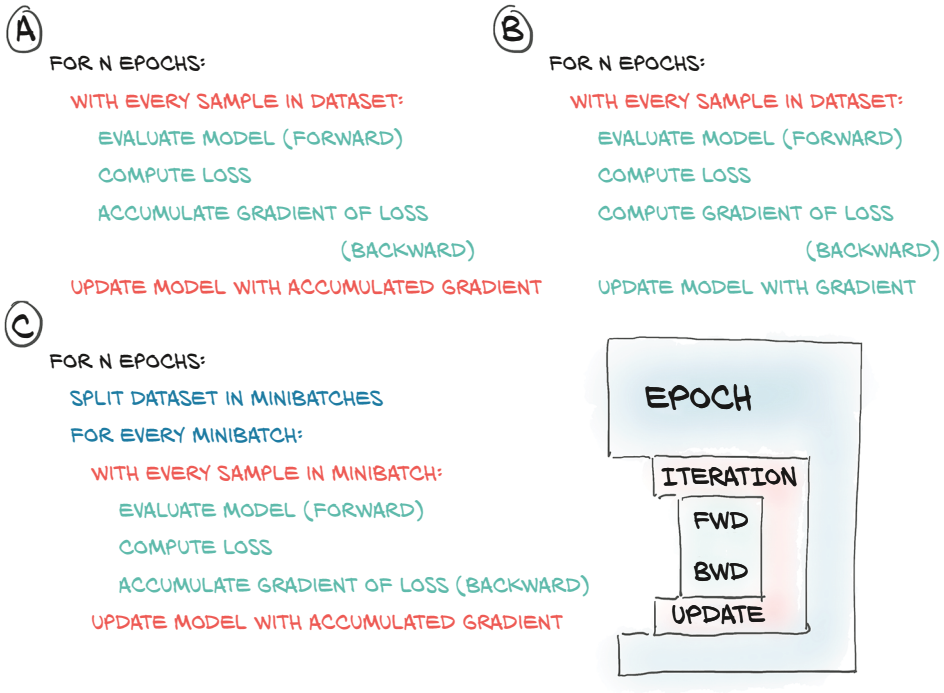


Figure 7.12 Training loops: (A) averaging updates over the whole dataset; (B) updating the model at each sample; (C) averaging updates over minibatches

Looking more closely, we made a small change to the training loop. In chapter 5, we had just one loop: over the epochs (recall that an epoch ends when all samples in the training set have been evaluated). We figured that evaluating all 10,000 images in a single batch would be too much, so we decided to have an inner loop where we evaluate one sample at a time and backpropagate over that single sample.

While in the first case the gradient is accumulated over all samples before being applied, in this case we apply changes to parameters based on a very partial estimation

of the gradient on a single sample. However, what is a good direction for reducing the loss based on one sample might not be a good direction for others. By shuffling samples at each epoch and estimating the gradient on one or (preferably, for stability) a few samples at a time, we are effectively introducing randomness in our gradient descent. Remember SGD? It stands for *stochastic gradient descent*, and this is what the *S* is about: working on small batches (aka minibatches) of shuffled data. It turns out that following gradients estimated over minibatches, which are poorer approximations of gradients estimated across the whole dataset, helps convergence and prevents the optimization process from getting stuck in local minima it encounters along the way. As depicted in figure 7.13, gradients from minibatches are randomly off the ideal trajectory, which is part of the reason why we want to use a reasonably small learning rate. Shuffling the dataset at each epoch helps ensure that the sequence of gradients estimated over minibatches is representative of the gradients computed across the full dataset.

Typically, minibatches are a constant size that we need to set prior to training, just like the learning rate. These are called *hyperparameters*, to distinguish them from the parameters of a model.

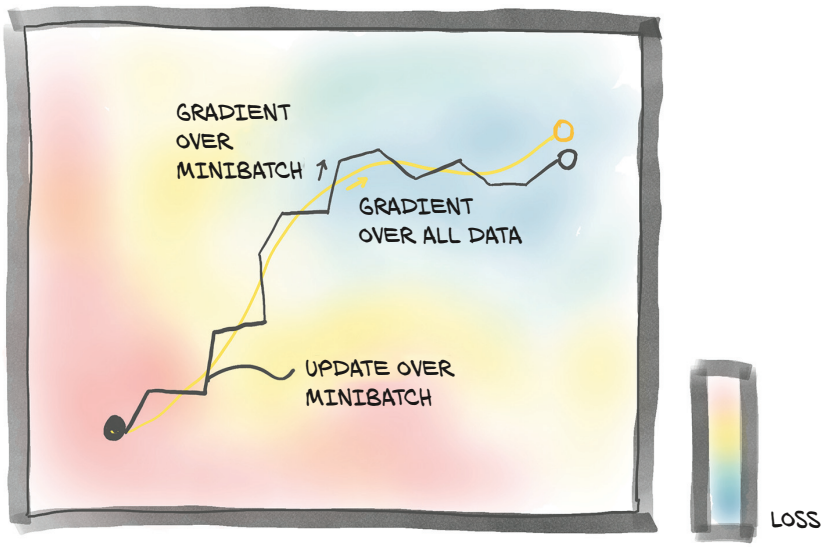


Figure 7.13 Gradient descent averaged over the whole dataset (light path) versus stochastic gradient descent, where the gradient is estimated on randomly picked minibatches

In our training code, we chose minibatches of size 1 by picking one item at a time from the dataset. The `torch.utils.data` module has a class that helps with shuffling and organizing the data in minibatches: `DataLoader`. The job of a data loader is to sample minibatches from a dataset, giving us the flexibility to choose from different sampling strategies. A very common strategy is uniform sampling after shuffling the data at each epoch. Figure 7.14 shows the data loader shuffling the indices it gets from the `Dataset`.

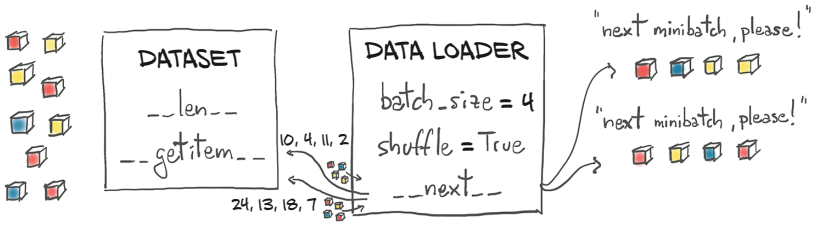


Figure 7.14 A data loader dispensing minibatches by using a dataset to sample individual data items

Let's see how this is done. At a minimum, the `DataLoader` constructor takes a `Dataset` object as input, along with `batch_size` and a `shuffle` Boolean that indicates whether the data needs to be shuffled at the beginning of each epoch:

```
train_loader = torch.utils.data.DataLoader(cifar2, batch_size=64,
                                           shuffle=True)
```

A `DataLoader` can be iterated over, so we can use it directly in the inner loop of our new training code:

```
import torch
import torch.nn as nn

train_loader = torch.utils.data.DataLoader(cifar2, batch_size=64,
                                           shuffle=True)

model = nn.Sequential(
            nn.Linear(3072, 512),
            nn.Tanh(),
            nn.Linear(512, 2),
            nn.LogSoftmax(dim=1))

learning_rate = 1e-2

optimizer = optim.SGD(model.parameters(), lr=learning_rate)

loss_fn = nn.NLLLoss()

n_epochs = 100

for epoch in range(n_epochs):
    for imgs, labels in train_loader:
```

```
        batch_size = imgs.shape[0]
        outputs = model(imgs.view(batch_size, -1))
        loss = loss_fn(outputs, labels)

        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

    print("Epoch: %d, Loss: %f" % (epoch, float(loss)))
```

Due to the shuffling, this now prints the loss for a random batch—clearly something we want to improve in chapter 8.

At each inner iteration, `imgs` is a tensor of size 64 × 3 × 32 × 32—that is, a minibatch of 64 (32 × 32) RGB images—while `labels` is a tensor of size 64 containing label indices.

Let's run our training:

```
Epoch: 0, Loss: 0.523478
Epoch: 1, Loss: 0.391083
Epoch: 2, Loss: 0.407412
Epoch: 3, Loss: 0.364203
...
Epoch: 96, Loss: 0.019537
Epoch: 97, Loss: 0.008973
Epoch: 98, Loss: 0.002607
Epoch: 99, Loss: 0.026200
```

We see that the loss decreases somehow, but we have no idea whether it's low enough. Since our goal here is to correctly assign classes to images, and preferably do that on an independent dataset, we can compute the accuracy of our model on the validation set in terms of the number of correct classifications over the total:

```
val_loader = torch.utils.data.DataLoader(cifar2_val, batch_size=64,
                                         shuffle=False)

correct = 0
total = 0

with torch.no_grad():
    for imgs, labels in val_loader:
        batch_size = imgs.shape[0]
        outputs = model(imgs.view(batch_size, -1))
        _, predicted = torch.max(outputs, dim=1)
        total += labels.shape[0]
        correct += int((predicted == labels).sum())

print("Accuracy: %f", correct / total)
```

```
Accuracy: 0.794000
```

Not a great performance, but quite a lot better than random. In our defense, our model was quite a shallow classifier; it's a miracle that it worked at all. It did because our dataset is really simple—a lot of the samples in the two classes likely have systematic differences (such as the color of the background) that help the model tell birds from airplanes, based on a few pixels.

We can certainly add some bling to our model by including more layers, which will increase the model's depth and capacity. One rather arbitrary possibility is

```
model = nn.Sequential(
            nn.Linear(3072, 1024),
            nn.Tanh(),
            nn.Linear(1024, 512),
            nn.Tanh(),
            nn.Linear(512, 128),
            nn.Tanh(),
            nn.Linear(128, 2),
            nn.LogSoftmax(dim=1))
```

Here we are trying to taper the number of features more gently toward the output, in the hope that intermediate layers will do a better job of squeezing information in increasingly shorter intermediate outputs.

The combination of `nn.LogSoftmax` and `nn.NLLLoss` is equivalent to using `nn.CrossEntropyLoss`. This terminology is a particularity of PyTorch, as the `nn.NLLoss` computes, in fact, the cross entropy but with log probability predictions as inputs where `nn.CrossEntropyLoss` takes scores (sometimes called *logits*). Technically, `nn.NLLLoss` is the cross entropy between the Dirac distribution, putting all mass on the target, and the predicted distribution given by the log probability inputs.

To add to the confusion, in information theory, up to normalization by sample size, this cross entropy can be interpreted as a negative log likelihood of the predicted distribution under the target distribution as an outcome. So both losses are the negative log likelihood of the model parameters given the data when our model predicts the (softmax-applied) probabilities. In this book, we won't rely on these details, but don't let the PyTorch naming confuse you when you see the terms used in the literature.

It is quite common to drop the last `nn.LogSoftmax` layer from the network and use `nn.CrossEntropyLoss` as a loss. Let us try that:

```
model = nn.Sequential(
            nn.Linear(3072, 1024),
            nn.Tanh(),
            nn.Linear(1024, 512),
            nn.Tanh(),
            nn.Linear(512, 128),
            nn.Tanh(),
            nn.Linear(128, 2))

loss_fn = nn.CrossEntropyLoss()
```

Note that the numbers will be *exactly* the same as with `nn.LogSoftmax` and `nn.NLLLoss`. It's just more convenient to do it all in one pass, with the only gotcha being that the output of our model will not be interpretable as probabilities (or log probabilities). We'll need to explicitly pass the output through a softmax to obtain those.

Training this model and evaluating the accuracy on the validation set (0.802000) lets us appreciate that a larger model bought us an increase in accuracy, but not that much. The accuracy on the training set is practically perfect (0.998100). What is this telling us? That we are overfitting our model in both cases. Our fully connected model is finding a way to discriminate birds and airplanes on the training set by memorizing the training set, but performance on the validation set is not all that great, even if we choose a larger model.

PyTorch offers a quick way to determine how many parameters a model has through the `parameters()` method of `nn.Model` (the same method we use to provide the parameters to the optimizer). To find out how many elements are in each tensor instance, we can call the `numel` method. Summing those gives us our total count. Depending on our use case, counting parameters might require us to check whether a parameter has `requires_grad` set to `True`, as well. We might want to differentiate the number of *trainable* parameters from the overall model size. Let's take a look at what we have right now:

```
# In[7]:
numel_list = [p.numel()
              for p in connected_model.parameters()
              if p.requires_grad == True]
sum(numel_list), numel_list

# Out[7]:
(3737474, [3145728, 1024, 524288, 512, 65536, 128, 256, 2])
```

Wow, 3.7 million parameters! Not a small network for such a small input image, is it? Even our first network was pretty large:

```
# In[9]:
numel_list = [p.numel() for p in first_model.parameters()]
sum(numel_list), numel_list

# Out[9]:
(1574402, [1572864, 512, 1024, 2])
```

The number of parameters in our first model is roughly half that in our latest model. Well, from the list of individual parameter sizes, we start having an idea what's responsible: the first module, which has 1.5 million parameters. In our full network, we had 1,024 output features, which led the first linear module to have 3 million parameters. This shouldn't be unexpected: we know that a linear layer computes `y = weight * x + bias`, and if `x` has length 3,072 (disregarding the batch dimension for simplicity) and `y` must have length 1,024, then the `weight` tensor needs to be of size 1,024 × 3,072 and the `bias` size must be 1,024. And 1,024 * 3,072 + 1,024 = 3,146,752, as we found earlier. We can verify these quantities directly:

```
# In[10]:
linear = nn.Linear(3072, 1024)

linear.weight.shape, linear.bias.shape

# Out[10]:
(torch.Size([1024, 3072]), torch.Size([1024]))
```

What is this telling us? That our neural network won't scale very well with the number of pixels. What if we had a 1,024 × 1,024 RGB image? That's 3.1 million input values. Even abruptly going to 1,024 hidden features (which is not going to work for our classifier), we would have over 3 *billion* parameters. Using 32-bit floats, we're already at 12 GB of RAM, and we haven't even hit the second layer, much less computed and stored the gradients. That's just not going to fit on most present-day GPUs.

7.2.7 The limits of going fully connected

Let's reason about what using a linear module on a 1D view of our image entails—figure 7.15 shows what is going on. It's like taking every single input value—that is, every single component in our RGB image—and computing a linear combination of it with all the other values for every output feature. On one hand, we are allowing for the combination of any pixel with every other pixel in the image being potentially relevant for our task. On the other hand, we aren't utilizing the relative position of neighboring or faraway pixels, since we are treating the image as one big vector of numbers.

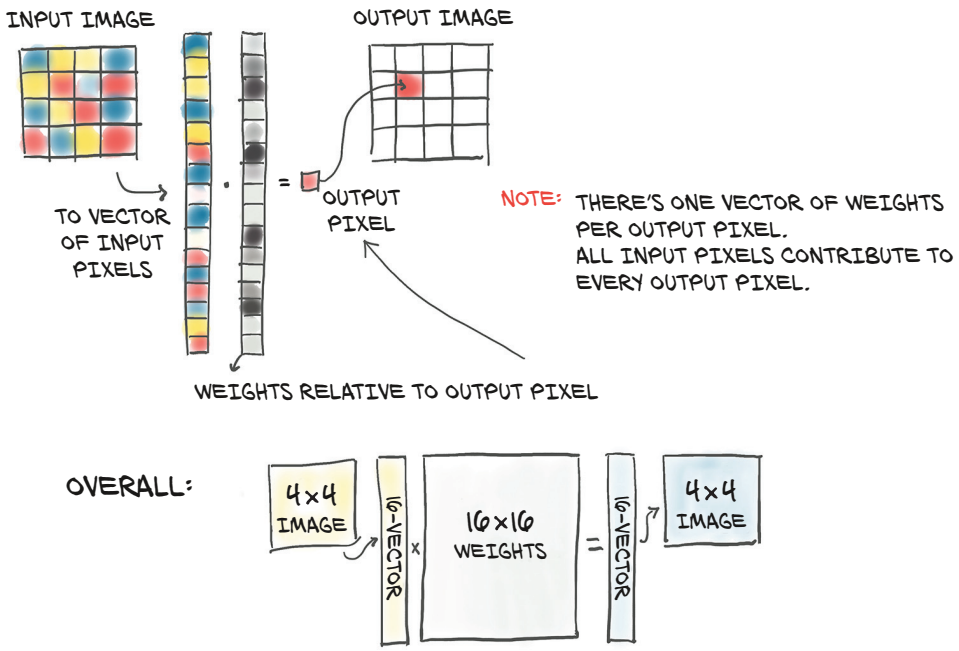


Figure 7.15 Using a fully connected module with an input image: every input pixel is combined with every other to produce each element in the output.

An airplane flying in the sky captured in a 32 × 32 image will be very roughly similar to a dark, cross-like shape on a blue background. A fully connected network as in figure 7.15 would need to learn that when pixel 0,1 is dark, pixel 1,1 is also dark, and so on, that's a good indication of an airplane. This is illustrated in the top half of figure 7.16. However, shift the same airplane by one pixel or more as in the bottom half of the figure, and the relationships between pixels will have to be relearned from scratch: this time, an airplane is likely when pixel 0,2 is dark, pixel 1,2 is dark, and so on. In more technical terms, a fully connected network is not *translation invariant*. This means a network that has been trained to recognize a Spitfire starting at position 4,4 will not be able to recognize the *exact same* Spitfire starting at position 8,8. We would then have to *augment* the dataset—that is, apply random translations to images during training—so the network would have a chance to see Spitfires all over the image, and we would need to do this for every image in the dataset (for the record, we could concatenate a

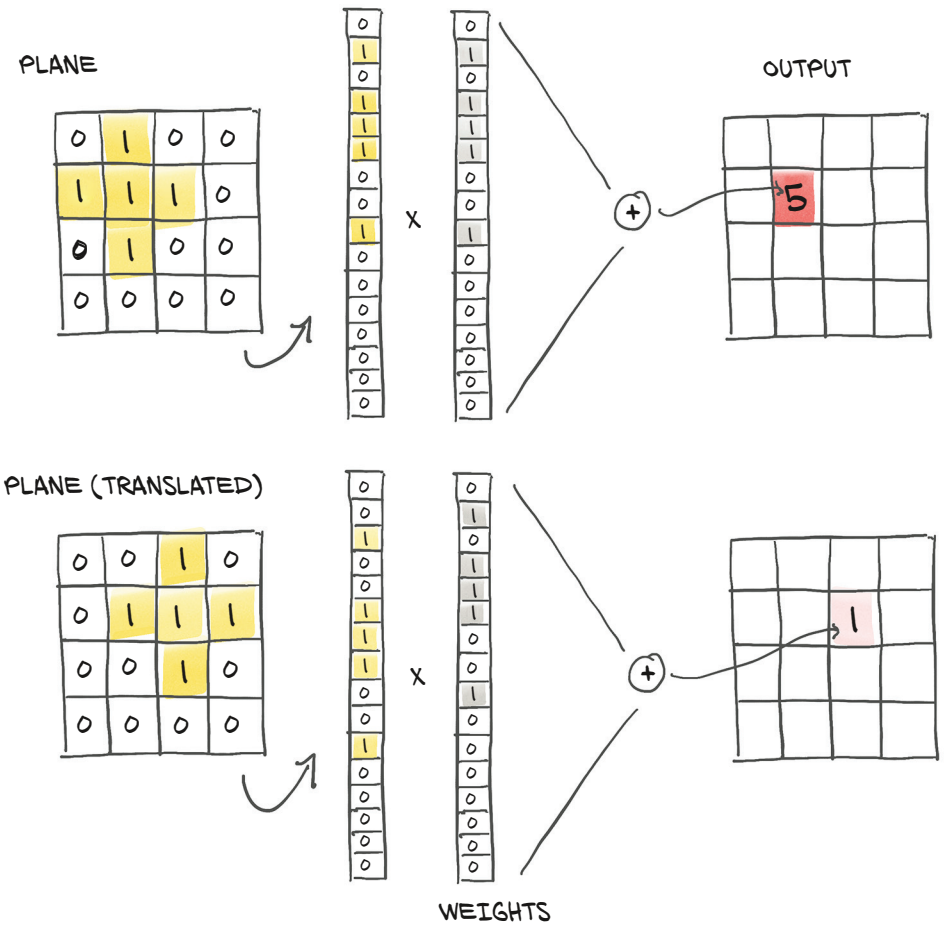


Figure 7.16 Translation invariance, or the lack thereof, with fully connected layers

transform from `torchvision.transforms` to do this transparently). However, this *data augmentation* strategy comes at a cost: the number of hidden features—that is, of parameters—must be large enough to store the information about all of these translated replicas.

So, at the end of this chapter, we have a dataset, a model, and a training loop, and our model learns. However, due to a mismatch between our problem and our network structure, we end up overfitting our training data, rather than learning the generalized features of what we want the model to detect.

We've created a model that allows for relating every pixel to every other pixel in the image, regardless of their spatial arrangement. We have a reasonable assumption that pixels that are closer together are in theory a lot more related, though. This means we are training a classifier that is not translation-invariant, so we're forced to use a lot of capacity for learning translated replicas if we want to hope to do well on the validation set. There has to be a better way, right?

Of course, most such questions in a book like this are rhetorical. The solution to our current set of problems is to change our model to use convolutional layers. We'll cover what that means in the next chapter.

7.3 Conclusion

In this chapter, we have solved a simple classification problem from dataset, to model, to minimizing an appropriate loss in a training loop. All of these things will be standard tools for your PyTorch toolbelt, and the skills needed to use them will be useful throughout your PyTorch tenure.

We've also found a severe shortcoming of our model: we have been treating 2D images as 1D data. Also, we do not have a natural way to incorporate the translation invariance of our problem. In the next chapter, you'll learn how to exploit the 2D nature of image data to get much better results.[9]

We could use what we have learned right away to process data without this translation invariance. For example, using it on tabular data or the time-series data we met in chapter 4, we can probably do great things already. To some extent, it would also be possible to use it on text data that is appropriately represented.[10]

7.4 Exercises

1. Use `torchvision` to implement random cropping of the data.
   a. How are the resulting images different from the uncropped originals?
   b. What happens when you request the same image a second time?
   c. What is the result of training using randomly cropped images?

[9] The same caveat about translation invariance also applies to purely 1D data: an audio classifier should likely produce the same output even if the sound to be classified starts a tenth of a second earlier or later.

[10] *Bag-of-words models*, which just average over word embeddings, can be processed with the network design from this chapter. More contemporary models take the positions of the words into account and need more advanced models.

2. Switch loss functions (perhaps MSE).
   a. Does the training behavior change?
3. Is it possible to reduce the capacity of the network enough that it stops overfitting?
   a. How does the model perform on the validation set when doing so?

7.5 Summary

- Computer vision is one of the most extensive applications of deep learning.
- Several datasets of annotated images are publicly available; many of them can be accessed via `torchvision`.
- `Datasets` and `DataLoaders` provide a simple yet effective abstraction for loading and sampling datasets.
- For a classification task, using the softmax function on the output of a network produces values that satisfy the requirements for being interpreted as probabilities. The ideal loss function for classification in this case is obtained by using the output of softmax as the input of a non-negative log likelihood function. The combination of softmax and such loss is called cross entropy in PyTorch.
- Nothing prevents us from treating images as vectors of pixel values, dealing with them using a fully connected network, just like any other numerical data. However, doing so makes it much harder to take advantage of the spatial relationships in the data.
- Simple models can be created using `nn.Sequential`.

8 Using convolutions to generalize

This chapter covers

- Understanding convolution
- Building a convolutional neural network
- Creating custom `nn.Module` subclasses
- The difference between the module and functional APIs
- Design choices for neural networks

In the previous chapter, we built a simple neural network that could fit (or overfit) the data, thanks to the many parameters available for optimization in the linear layers. We had issues with our model, however, in that it was better at memorizing the training set than it was at generalizing properties of birds and airplanes. Based on our model architecture, we've got a guess as to why that's the case. Due to the fully connected setup needed to detect the various possible translations of the bird or airplane in the image, we have both too many parameters (making it easier for the model to memorize the training set) and no position independence (making it harder to generalize). As we discussed in the last chapter, we could augment our

training data by using a wide variety of recropped images to try to force generalization, but that won't address the issue of having too many parameters.

There is a better way! It consists of replacing the dense, fully connected affine transformation in our neural network unit with a different linear operation: convolution.

8.1 The case for convolutions

Let's get to the bottom of what convolutions are and how we can use them in our neural networks. Yes, yes, we were in the middle of our quest to tell birds from airplanes, and our friend is still waiting for our solution, but this diversion is worth the extra time spent. We'll develop an intuition for this foundational concept in computer vision and then return to our problem equipped with superpowers.

In this section, we'll see how convolutions deliver locality and translation invariance. We'll do so by taking a close look at the formula defining convolutions and applying it using pen and paper—but don't worry, the gist will be in pictures, not formulas.

We said earlier that taking a 1D view of our input image and multiplying it by an `n_output_features × n_input_features` weight matrix, as is done in `nn.Linear`, means for each channel in the image, computing a weighted sum of all the pixels multiplied by a set of weights, one per output feature.

We also said that, if we want to recognize patterns corresponding to objects, like an airplane in the sky, we will likely need to look at how nearby pixels are arranged, and we will be less interested in how pixels that are far from each other appear in combination. Essentially, it doesn't matter if our image of a Spitfire has a tree or cloud or kite in the corner or not.

In order to translate this intuition into mathematical form, we could compute the weighted sum of a pixel with its immediate neighbors, rather than with all other pixels in the image. This would be equivalent to building weight matrices, one per output feature and output pixel location, in which all weights beyond a certain distance from a center pixel are zero. This will still be a weighted sum: that is, a linear operation.

8.1.1 What convolutions do

We identified one more desired property earlier: we would like these localized patterns to have an effect on the output regardless of their location in the image: that is, to be *translation invariant*. To achieve this goal in a matrix applied to the image-as-a-vector we used in chapter 7 would require implementing a rather complicated pattern of weights (don't worry if it is *too* complicated; it'll get better shortly): most of the weight matrix would be zero (for entries corresponding to input pixels too far away from the output pixel to have an influence). For other weights, we would have to find a way to keep entries in sync that correspond to the same relative position of input and output pixels. This means we would need to initialize them to the same values and ensure that all these *tied* weights stayed the same while the network is updated during training. This way, we would ensure that weights operate in neighborhoods to respond to local patterns, and local patterns are identified no matter where they occur in the image.

Of course, this approach is more than impractical. Fortunately, there is a readily available, local, translation-invariant linear operation on the image: a *convolution*. We can come up with a more compact description of a convolution, but what we are going to describe is exactly what we just delineated—only taken from a different angle.

Convolution, or more precisely, *discrete convolution*[1] (there's an analogous continuous version that we won't go into here), is defined for a 2D image as the scalar product of a weight matrix, the *kernel*, with every neighborhood in the input. Consider a 3×3 kernel (in deep learning, we typically use small kernels; we'll see why later on) as a 2D tensor

```
weight = torch.tensor([[w00, w01, w02],
                       [w10, w11, w12],
                       [w20, w21, w22]])
```

and a 1-channel, MxN image:

```
image = torch.tensor([[i00, i01, i02, i03, ..., i0N],
                      [i10, i11, i12, i13, ..., i1N],
                      [i20, i21, i22, i23, ..., i2N],
                      [i30, i31, i32, i33, ..., i3N],
                      ...
                      [iM0, iM1m iM2, iM3, ..., iMN]])
```

We can compute an element of the output image (without bias) as follows:

```
o11 = i11 * w00 + i12 * w01 + i22 * w02 +
      i21 * w10 + i22 * w11 + i23 * w12 +
      i31 * w20 + i32 * w21 + i33 * w22
```

Figure 8.1 shows this computation in action.

That is, we "translate" the kernel on the `i11` location of the input image, and we multiply each weight by the value of the input image at the corresponding location. Thus, the output image is created by translating the kernel on all input locations and performing the weighted sum. For a multichannel image, like our RGB image, the weight matrix would be a $3 \times 3 \times 3$ matrix: one set of weights for every channel, contributing together to the output values.

Note that, just like the elements in the `weight` matrix of `nn.Linear`, the weights in the kernel are not known in advance, but they are initialized randomly and updated through backpropagation. Note also that the same kernel, and thus each weight in the kernel, is reused across the whole image. Thinking back to autograd, this means the use of each weight has a history spanning the entire image. Thus, the derivative of the loss with respect to a convolution weight includes contributions from the entire image.

[1] There is a subtle difference between PyTorch's convolution and mathematics' convolution: one argument's sign is flipped. If we were in a pedantic mood, we could call PyTorch's convolutions *discrete cross-correlations*.

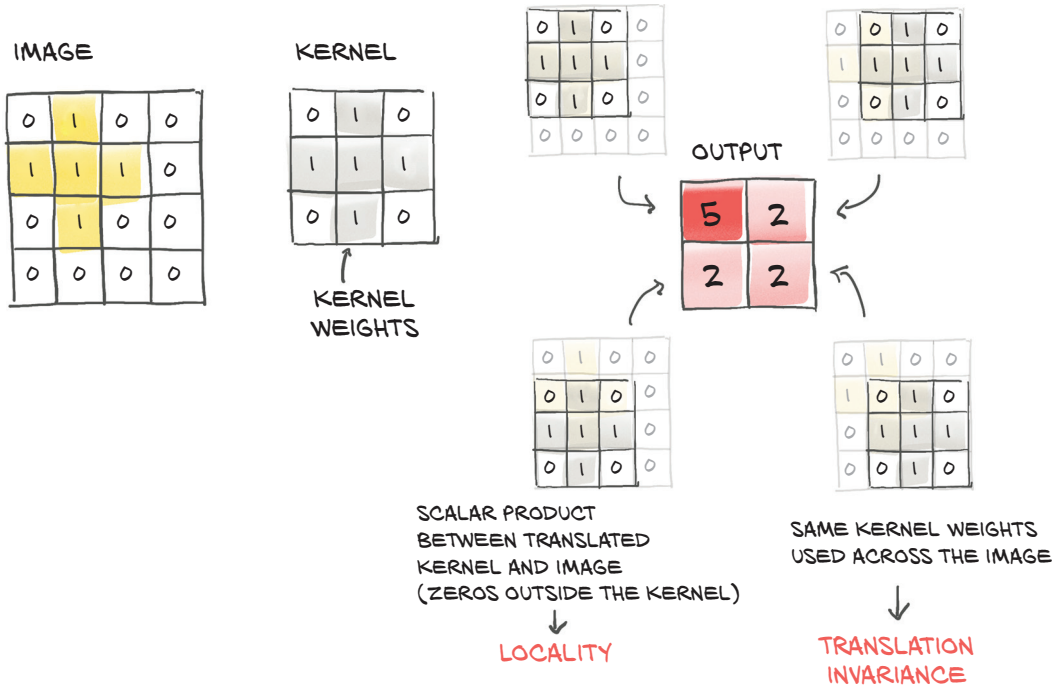


Figure 8.1 Convolution: locality and translation invariance

It's now possible to see the connection to what we were stating earlier: a convolution is equivalent to having multiple linear operations whose weights are zero almost everywhere except around individual pixels and that receive equal updates during training.

Summarizing, by switching to convolutions, we get

- Local operations on neighborhoods
- Translation invariance
- Models with a lot fewer parameters

The key insight underlying the third point is that, with a convolution layer, the number of parameters depends not on the number of pixels in the image, as was the case in our fully connected model, but rather on the size of the convolution kernel (3×3, 5×5, and so on) and on how many convolution filters (or output channels) we decide to use in our model.

8.2 Convolutions in action

Well, it looks like we've spent enough time down a rabbit hole! Let's see some PyTorch in action on our birds versus airplanes challenge. The `torch.nn` module provides convolutions for 1, 2, and 3 dimensions: `nn.Conv1d` for time series, `nn.Conv2d` for images, and `nn.Conv3d` for volumes or videos.

For our CIFAR-10 data, we'll resort to `nn.Conv2d`. At a minimum, the arguments we provide to `nn.Conv2d` are the number of input features (or *channels*, since we're dealing

with *multichannel* images: that is, more than one value per pixel), the number of output features, and the size of the kernel. For instance, for our first convolutional module, we'll have 3 input features per pixel (the RGB channels) and an arbitrary number of channels in the output—say, 16. The more channels in the output image, the more the capacity of the network. We need the channels to be able to detect many different types of features. Also, because we are randomly initializing them, some of the features we'll get, even after training, will turn out to be useless.[2] Let's stick to a kernel size of 3 × 3.

It is very common to have kernel sizes that are the same in all directions, so PyTorch has a shortcut for this: whenever `kernel_size=3` is specified for a 2D convolution, it means 3 × 3 (provided as a tuple `(3, 3)` in Python). For a 3D convolution, it means 3 × 3 × 3. The CT scans we will see in part 2 of the book have a different voxel (volumetric pixel) resolution in one of the three axes. In such a case, it makes sense to consider kernels that have a different size for the exceptional dimension. But for now, we stick with having the same size of convolutions across all dimensions:

```
# In[11]:
conv = nn.Conv2d(3, 16, kernel_size=3)
conv

# Out[11]:
Conv2d(3, 16, kernel_size=(3, 3), stride=(1, 1))
```

Instead of the shortcut kernel_size=3, we could equivalently pass in the tuple that we see in the output: kernel_size=(3, 3).

What do we expect to be the shape of the `weight` tensor? The kernel is of size 3 × 3, so we want the weight to consist of 3 × 3 parts. For a single output pixel value, our kernel would consider, say, `in_ch` = 3 input channels, so the weight component for a single output pixel value (and by translation the invariance for the entire output channel) is of shape `in_ch` × 3 × 3. Finally, we have as many of those as we have output channels, here `out_ch` = 16, so the complete weight tensor is `out_ch` × `in_ch` × 3 × 3, in our case 16 × 3 × 3 × 3. The bias will have size 16 (we haven't talked about bias for a while for simplicity, but just as in the linear module case, it's a constant value we add to each channel of the output image). Let's verify our assumptions:

```
# In[12]:
conv.weight.shape, conv.bias.shape

# Out[12]:
(torch.Size([16, 3, 3, 3]), torch.Size([16]))
```

We can see how convolutions are a convenient choice for learning from images. We have smaller models looking for local patterns whose weights are optimized across the entire image.

A 2D convolution pass produces a 2D image as output, whose pixels are a weighted sum over neighborhoods of the input image. In our case, both the kernel weights and

[2] This is part of the *lottery ticket hypothesis*: that many kernels will be as useful as losing lottery tickets. See Jonathan Frankle and Michael Carbin, "The Lottery Ticket Hypothesis: Finding Sparse, Trainable Neural Networks," 2019, https://arxiv.org/abs/1803.03635.

the bias `conv.weight` are initialized randomly, so the output image will not be particularly meaningful. As usual, we need to add the zeroth batch dimension with `unsqueeze` if we want to call the `conv` module with one input image, since `nn.Conv2d` expects a $B \times C \times H \times W$ shaped tensor as input:

```
# In[13]:
img, _ = cifar2[0]
output = conv(img.unsqueeze(0))
img.unsqueeze(0).shape, output.shape

# Out[13]:
(torch.Size([1, 3, 32, 32]), torch.Size([1, 16, 30, 30]))
```

We're curious, so we can display the output, shown in figure 8.2:

```
# In[15]:
plt.imshow(output[0, 0].detach(), cmap='gray')
plt.show()
```

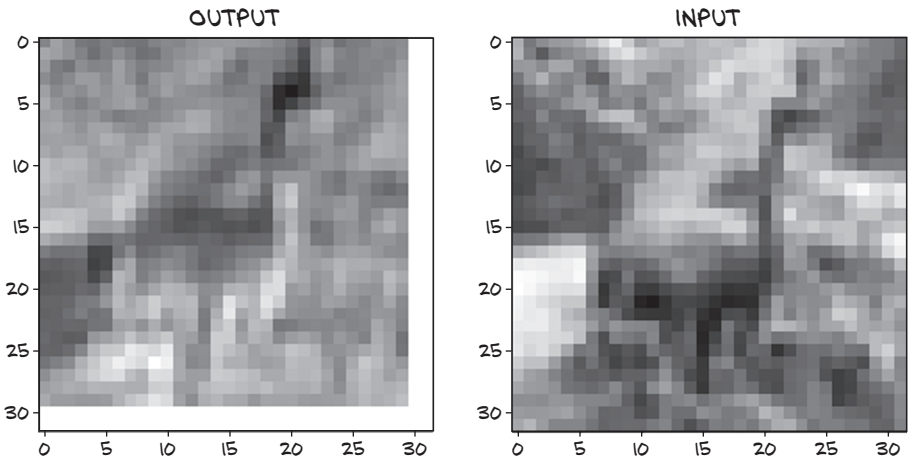


Figure 8.2 Our bird after a random convolution treatment. (We cheated a little with the code to show you the input, too.)

Wait a minute. Let's take a look a the size of `output`: it's `torch.Size([1, 16, 30, 30])`. Huh; we lost a few pixels in the process. How did that happen?

8.2.1 Padding the boundary

The fact that our output image is smaller than the input is a side effect of deciding what to do at the boundary of the image. Applying a convolution kernel as a weighted sum of pixels in a 3×3 neighborhood requires that there are neighbors in all directions. If we are at i00, we only have pixels to the right of and below us. By default, PyTorch will slide the convolution kernel within the input picture, getting `width - kernel_width + 1` horizontal and vertical positions. For odd-sized kernels, this results in images that are

one-half the convolution kernel's width (in our case, 3//2 = 1) smaller on each side. This explains why we're missing two pixels in each dimension.

However, PyTorch gives us the possibility of *padding* the image by creating *ghost* pixels around the border that have value zero as far as the convolution is concerned. Figure 8.3 shows padding in action.

In our case, specifying `padding=1` when `kernel_size=3` means i00 has an extra set of neighbors above it and to its left, so that an output of the convolution can be computed even in the corner of our original image.[3] The net result is that the output has now the exact same size as the input:

```
# In[16]:
conv = nn.Conv2d(3, 1, kernel_size=3, padding=1)      <-- Now with padding
output = conv(img.unsqueeze(0))
img.unsqueeze(0).shape, output.shape

# Out[16]:
(torch.Size([1, 3, 32, 32]), torch.Size([1, 1, 32, 32]))
```

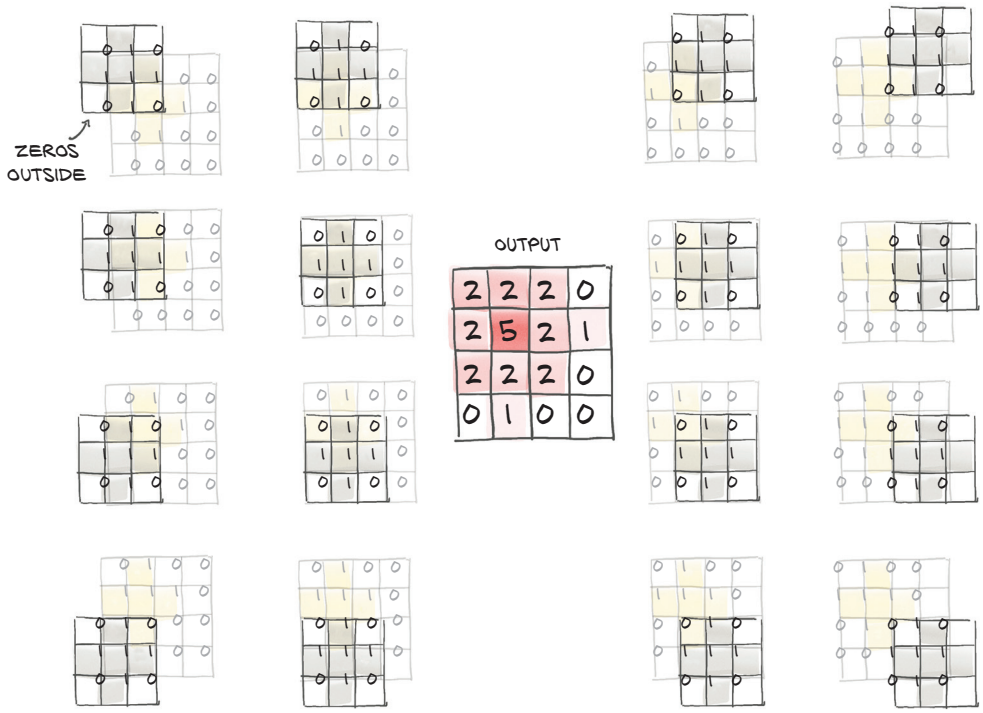


Figure 8.3 Zero padding to preserve the image size in the output

[3] For even-sized kernels, we would need to pad by a different number on the left and right (and top and bottom). PyTorch doesn't offer to do this in the convolution itself, but the function `torch.nn.functional.pad` can take care of it. But it's best to stay with odd kernel sizes; even-sized kernels are just odd.

Note that the sizes of `weight` and `bias` don't change, regardless of whether padding is used.

There are two main reasons to pad convolutions. First, doing so helps us separate the matters of convolution and changing image sizes, so we have one less thing to remember. And second, when we have more elaborate structures such as skip connections (discussed in section 8.5.3) or the U-Nets we'll cover in part 2, we want the tensors before and after a few convolutions to be of compatible size so that we can add them or take differences.

8.2.2 Detecting features with convolutions

We said earlier that `weight` and `bias` are parameters that are learned through backpropagation, exactly as it happens for `weight` and `bias` in `nn.Linear`. However, we can play with convolution by setting weights by hand and see what happens.

Let's first zero out `bias`, just to remove any confounding factors, and then set `weights` to a constant value so that each pixel in the output gets the mean of its neighbors. For each 3×3 neighborhood:

```
# In[17]:
with torch.no_grad():
    conv.bias.zero_()

with torch.no_grad():
    conv.weight.fill_(1.0 / 9.0)
```

We could have gone with `conv.weight.one_()`—that would result in each pixel in the output being the *sum* of the pixels in the neighborhood. Not a big difference, except that the values in the output image would have been nine times larger.

Anyway, let's see the effect on our CIFAR image:

```
# In[18]:
output = conv(img.unsqueeze(0))
plt.imshow(output[0, 0].detach(), cmap='gray')
plt.show()
```

As we could have predicted, the filter produces a blurred version of the image, as shown in figure 8.4. After all, every pixel of the output is the average of a neighborhood of the input, so pixels in the output are correlated and change more smoothly.

Next, let's try something different. The following kernel may look a bit mysterious at first:

```
# In[19]:
conv = nn.Conv2d(3, 1, kernel_size=3, padding=1)

with torch.no_grad():
    conv.weight[:] = torch.tensor([[-1.0, 0.0, 1.0],
                                   [-1.0, 0.0, 1.0],
                                   [-1.0, 0.0, 1.0]])
    conv.bias.zero_()
```

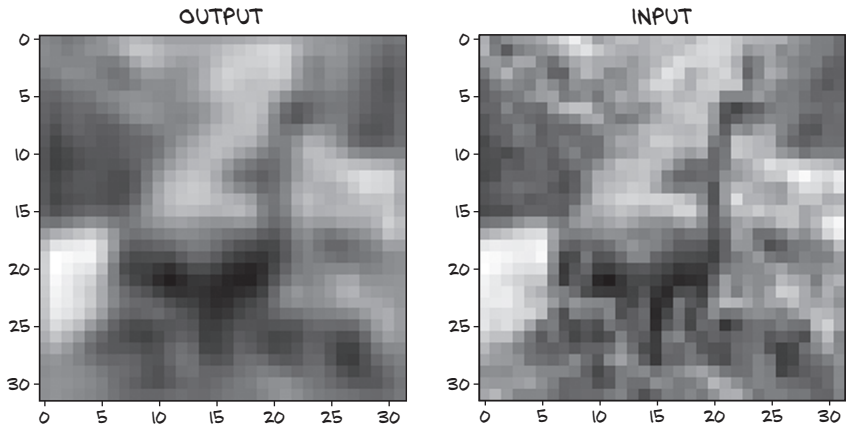


Figure 8.4 Our bird, this time blurred thanks to a constant convolution kernel

Working out the weighted sum for an arbitrary pixel in position 2,2, as we did earlier for the generic convolution kernel, we get

```
o22 = i13 - i11 +
      i23 - i21 +
      i33 - i31
```

which performs the difference of all pixels on the right of i22 minus the pixels on the left of i22. If the kernel is applied on a vertical boundary between two adjacent regions of different intensity, o22 will have a high value. If the kernel is applied on a region of uniform intensity, o22 will be zero. It's an *edge-detection* kernel: the kernel highlights the vertical edge between two horizontally adjacent regions.

Applying the convolution kernel to our image, we see the result shown in figure 8.5. As expected, the convolution kernel enhances the vertical edges. We could build

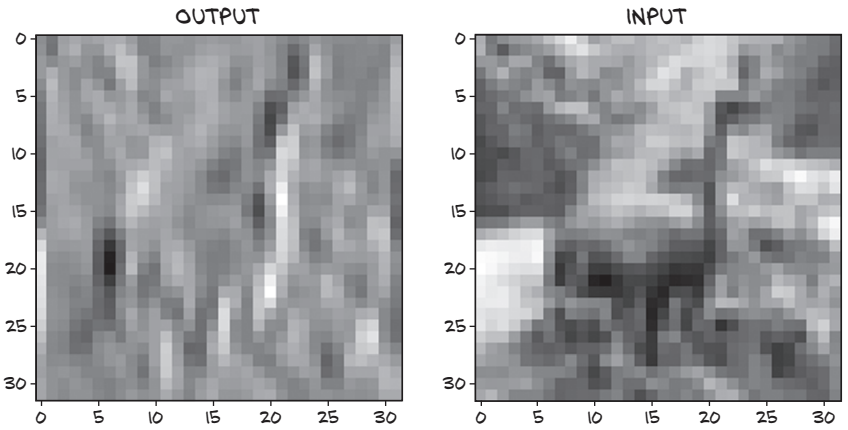


Figure 8.5 Vertical edges throughout our bird, courtesy of a handcrafted convolution kernel

lots more elaborate filters, such as for detecting horizontal or diagonal edges, or cross-like or checkerboard patterns, where "detecting" means the output has a high magnitude. In fact, the job of a computer vision expert has historically been to come up with the most effective combination of filters so that certain features are highlighted in images and objects can be recognized.

With deep learning, we let kernels be estimated from data in whatever way the discrimination is most effective: for instance, in terms of minimizing the negative cross-entropy loss between the output and the ground truth that we introduced in section 7.2.5. From this angle, the job of a convolutional neural network is to estimate the kernel of a set of filter banks in successive layers that will transform a multichannel image into another multichannel image, where different channels correspond to different features (such as one channel for the average, another channel for vertical edges, and so on). Figure 8.6 shows how the training automatically learns the kernels.

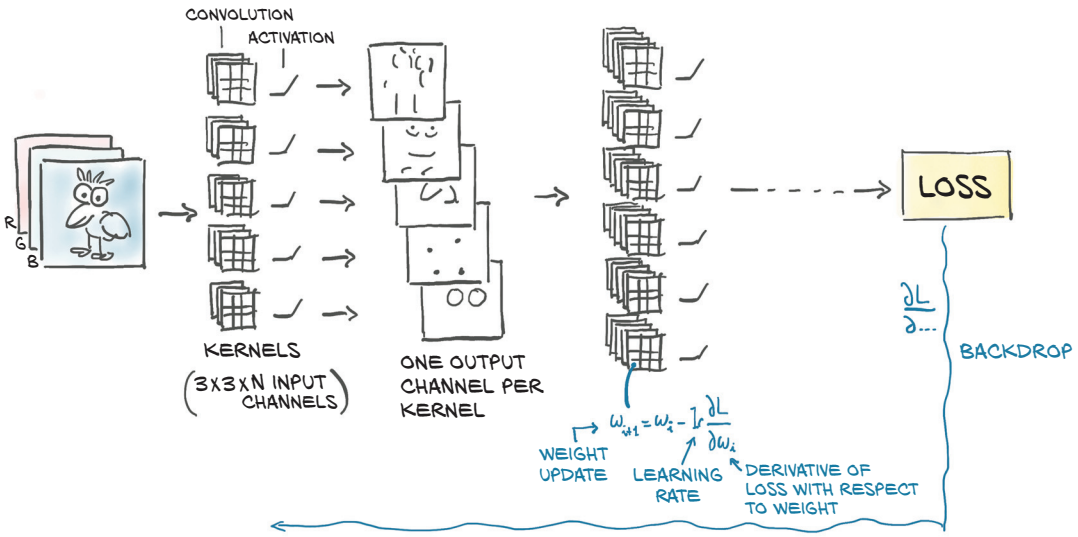


Figure 8.6 The process of learning with convolutions by estimating the gradient at the kernel weights and updating them individually in order to optimize for the loss

8.2.3 Looking further with depth and pooling

This is all well and good, but conceptually there's an elephant in the room. We got all excited because by moving from fully connected layers to convolutions, we achieve locality and translation invariance. Then we recommended the use of small kernels, like 3×3, or 5×5: that's peak locality, all right. What about the *big picture*? How do we know that all structures in our images are 3 pixels or 5 pixels wide? Well, we don't, because they aren't. And if they aren't, how are our networks going to be equipped to see those patterns with larger scope? This is something we'll really need if we want to

solve our birds versus airplanes problem effectively, since although CIFAR-10 images are small, the objects still have a (wing-)span several pixels across.

One possibility could be to use large convolution kernels. Well, sure, at the limit we could get a 32 × 32 kernel for a 32 × 32 image, but we would converge to the old fully connected, affine transformation and lose all the nice properties of convolution. Another option, which is used in convolutional neural networks, is stacking one convolution after the other and at the same time downsampling the image between successive convolutions.

FROM LARGE TO SMALL: DOWNSAMPLING

Downsampling could in principle occur in different ways. Scaling an image by half is the equivalent of taking four neighboring pixels as input and producing one pixel as output. How we compute the value of the output based on the values of the input is up to us. We could

- *Average the four pixels.* This *average pooling* was a common approach early on but has fallen out of favor somewhat.
- *Take the maximum of the four pixels.* This approach, called *max pooling,* is currently the most commonly used approach, but it has a downside of discarding the other three-quarters of the data.
- *Perform a strided convolution, where only every Nth pixel is calculated.* A 3 × 4 convolution with stride 2 still incorporates input from all pixels from the previous layer. The literature shows promise for this approach, but it has not yet supplanted max pooling.

We will be focusing on max pooling, illustrated in figure 8.7, going forward. The figure shows the most common setup of taking non-overlapping 2 x 2 tiles and taking the maximum over each of them as the new pixel at the reduced scale.

Intuitively, the output images from a convolution layer, especially since they are followed by an activation just like any other linear layer, tend to have a high magnitude

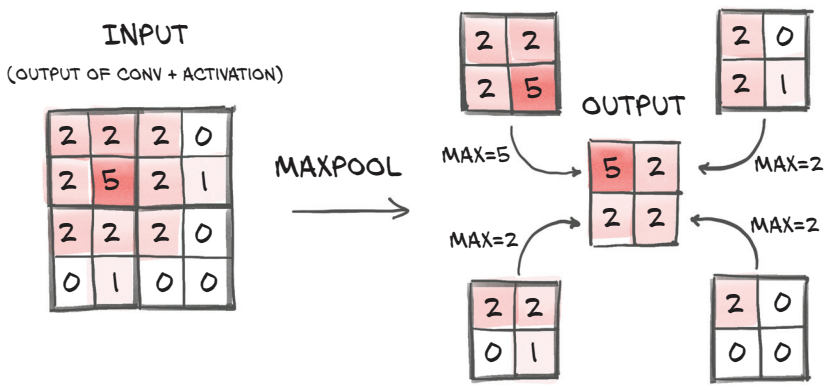


Figure 8.7 Max pooling in detail

where certain features corresponding to the estimated kernel are detected (such as vertical lines). By keeping the highest value in the 2 × 2 neighborhood as the downsampled output, we ensure that the features that are found *survive* the downsampling, at the expense of the weaker responses.

Max pooling is provided by the `nn.MaxPool2d` module (as with convolution, there are versions for 1D and 3D data). It takes as input the size of the neighborhood over which to operate the pooling operation. If we wish to downsample our image by half, we'll want to use a size of 2. Let's verify that it works as expected directly on our input image:

```
# In[21]:
pool = nn.MaxPool2d(2)
output = pool(img.unsqueeze(0))

img.unsqueeze(0).shape, output.shape

# Out[21]:
(torch.Size([1, 3, 32, 32]), torch.Size([1, 3, 16, 16]))
```

COMBINING CONVOLUTIONS AND DOWNSAMPLING FOR GREAT GOOD

Let's now see how combining convolutions and downsampling can help us recognize larger structures. In figure 8.8, we start by applying a set of 3 × 3 kernels on our 8 × 8 image, obtaining a multichannel output image of the same size. Then we scale down the output image by half, obtaining a 4 × 4 image, and apply another set of 3 × 3 kernels to it. This second set of kernels operates on a 3 × 3 neighborhood of something that has been scaled down by half, so it effectively maps back to 8 × 8 neighborhoods of the input. In addition, the second set of kernels takes the output of the first set of kernels (features like averages, edges, and so on) and extracts additional features on top of those.

So, on one hand, the first set of kernels operates on small neighborhoods on first-order, low-level features, while the second set of kernels effectively operates on wider neighborhoods, producing features that are compositions of the previous features. This is a very powerful mechanism that provides convolutional neural networks with the ability to see into very complex scenes—much more complex than our 32 × 32 images from the CIFAR-10 dataset.

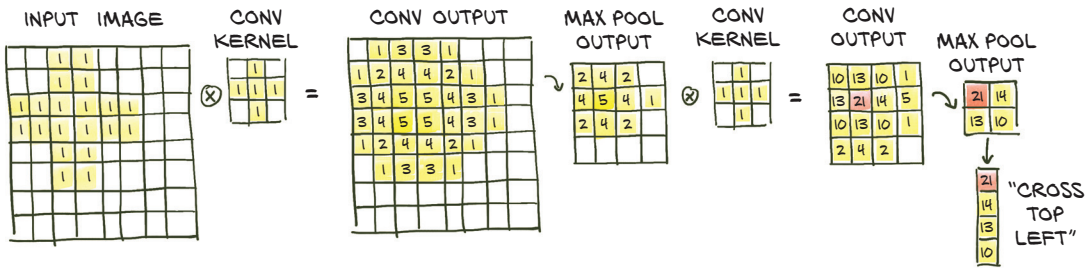


Figure 8.8 More convolutions by hand, showing the effect of stacking convolutions and downsampling: a large cross is highlighted using two small, cross-shaped kernels and max pooling.

The receptive field of output pixels

When the second 3 × 3 convolution kernel produces 21 in its conv output in figure 8.8, this is based on the top-left 3 × 3 pixels of the first max pool output. They, in turn, correspond to the 6 × 6 pixels in the top-left corner in the first conv output, which in turn are computed by the first convolution from the top-left 7 × 7 pixels. So the pixel in the second convolution output is influenced by a 7 × 7 input square. The first convolution also uses an implicitly "padded" column and row to produce the output in the corner; otherwise, we would have an 8 × 8 square of input pixels informing a given pixel (away from the boundary) in the second convolution's output. In fancy language, we say that a given output neuron of the 3 × 3-conv, 2 × 2-max-pool, 3 × 3-conv construction has a *receptive field* of 8 × 8.

8.2.4 Putting it all together for our network

With these building blocks in our hands, we can now proceed to build our convolutional neural network for detecting birds and airplanes. Let's take our previous fully connected model as a starting point and introduce `nn.Conv2d` and `nn.MaxPool2d` as described previously:

```
# In[22]:
model = nn.Sequential(
            nn.Conv2d(3, 16, kernel_size=3, padding=1),
            nn.Tanh(),
            nn.MaxPool2d(2),
            nn.Conv2d(16, 8, kernel_size=3, padding=1),
            nn.Tanh(),
            nn.MaxPool2d(2),
            # ...
            )
```

The first convolution takes us from 3 RGB channels to 16, thereby giving the network a chance to generate 16 independent features that operate to (hopefully) discriminate low-level features of birds and airplanes. Then we apply the `Tanh` activation function. The resulting 16-channel 32 × 32 image is pooled to a 16-channel 16 × 16 image by the first `MaxPool3d`. At this point, the downsampled image undergoes another convolution that generates an 8-channel 16 × 16 output. With any luck, this output will consist of higher-level features. Again, we apply a `Tanh` activation and then pool to an 8-channel 8 × 8 output.

Where does this end? After the input image has been reduced to a set of 8 × 8 features, we expect to be able to output some probabilities from the network that we can feed to our negative log likelihood. However, probabilities are a pair of numbers in a 1D vector (one for airplane, one for bird), but here we're still dealing with multichannel 2D features.

Thinking back to the beginning of this chapter, we already know what we need to do: turn the 8-channel 8 × 8 image into a 1D vector and complete our network with a set of fully connected layers:

```
# In[23]:
model = nn.Sequential(
            nn.Conv2d(3, 16, kernel_size=3, padding=1),
            nn.Tanh(),
            nn.MaxPool2d(2),
            nn.Conv2d(16, 8, kernel_size=3, padding=1),
            nn.Tanh(),
            nn.MaxPool2d(2),
            # ...
            nn.Linear(8 * 8 * 8, 32),
            nn.Tanh(),
            nn.Linear(32, 2))
```

Warning: Something important is missing here!

This code gives us a neural network as shown in figure 8.9.

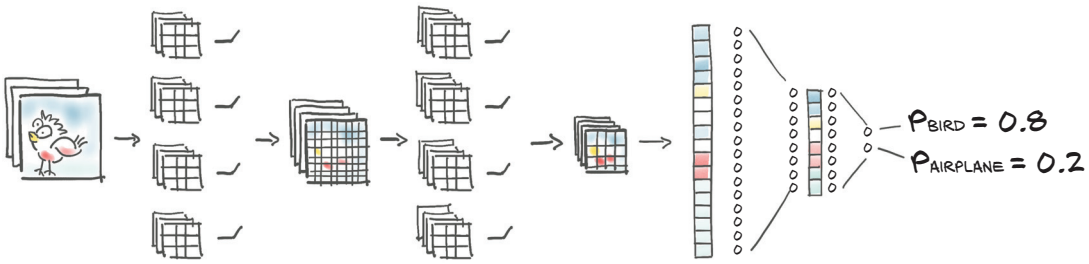


Figure 8.9 Shape of a typical convolutional network, including the one we're building. An image is fed to a series of convolutions and max pooling modules and then straightened into a 1D vector and fed into fully connected modules.

Ignore the "something missing" comment for a minute. Let's first notice that the size of the linear layer is dependent on the expected size of the output of `MaxPool2d`: 8 × 8 × 8 = 512. Let's count the number of parameters for this small model:

```
# In[24]:
numel_list = [p.numel() for p in model.parameters()]
sum(numel_list), numel_list

# Out[24]:
(18090, [432, 16, 1152, 8, 16384, 32, 64, 2])
```

That's very reasonable for a limited dataset of such small images. In order to increase the capacity of the model, we could increase the number of output channels for the convolution layers (that is, the number of features each convolution layer generates), which would lead the linear layer to increase its size as well.

We put the "Warning" note in the code for a reason. The model has zero chance of running without complaining:

```
# In[25]:
model(img.unsqueeze(0))

# Out[25]:
...
RuntimeError: size mismatch, m1:
➥ [64 x 8], m2: [512 x 32] at c:\...\THTensorMath.cpp:940
```

Admittedly, the error message is a bit obscure, but not too much so. We find references to `linear` in the traceback: looking back at the model, we see that only module that has to have a 512 × 32 tensor is `nn.Linear(512, 32)`, the first linear module after the last convolution block.

What's missing there is the reshaping step from an 8-channel 8 × 8 image to a 512-element, 1D vector (1D if we ignore the batch dimension, that is). This could be achieved by calling `view` on the output of the last `nn.MaxPool2d`, but unfortunately, we don't have any explicit visibility of the output of each module when we use `nn.Sequential`.[4]

8.3 Subclassing nn.Module

At some point in developing neural networks, we will find ourselves in a situation where we want to compute something that the premade modules do not cover. Here, it is something very simple like reshaping,[5]; but in section 8.5.3, we use the same construction to implement residual connections. So in this section, we learn how to make our own `nn.Module` subclasses that we can then use just like the prebuilt ones or `nn.Sequential`.

When we want to build models that do more complex things than just applying one layer after another, we need to leave `nn.Sequential` for something that gives us added flexibility. PyTorch allows us to use any computation in our model by subclassing `nn.Module`.

In order to subclass `nn.Module`, at a minimum we need to define a `forward` function that takes the inputs to the module and returns the output. This is where we define our module's computation. The name `forward` here is reminiscent of a distant past, when modules needed to define both the forward and backward passes we met in section 5.5.1. With PyTorch, if we use standard `torch` operations, autograd will take care of the backward pass automatically; and indeed, an `nn.Module` never comes with a `backward`.

Typically, our computation will use other modules—premade like convolutions or customized. To include these *submodules*, we typically define them in the constructor `__init__` and assign them to `self` for use in the `forward` function. They will, at the same time, hold their parameters throughout the lifetime of our module. Note that you need to call `super().__init__()` before you can do that (or PyTorch will remind you).

---

[4] Not being able to do this kind of operation inside of `nn.Sequential` was an explicit design choice by the PyTorch authors and was left that way for a long time; see the linked comments from @soumith at https://github.com/pytorch/pytorch/issues/2486. Recently, PyTorch gained an `nn.Flatten` layer.

[5] We could have used `nn.Flatten` starting from PyTorch 1.3.

8.3.1 Our network as an nn.Module

Let's write our network as a submodule. To do so, we instantiate all the `nn.Conv2d`, `nn.Linear`, and so on that we previously passed to `nn.Sequential` in the constructor, and then use their instances one after another in `forward`:

```
# In[26]:
class Net(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(3, 16, kernel_size=3, padding=1)
        self.act1 = nn.Tanh()
        self.pool1 = nn.MaxPool2d(2)
        self.conv2 = nn.Conv2d(16, 8, kernel_size=3, padding=1)
        self.act2 = nn.Tanh()
        self.pool2 = nn.MaxPool2d(2)
        self.fc1 = nn.Linear(8 * 8 * 8, 32)
        self.act3 = nn.Tanh()
        self.fc2 = nn.Linear(32, 2)

    def forward(self, x):
        out = self.pool1(self.act1(self.conv1(x)))
        out = self.pool2(self.act2(self.conv2(out)))
        out = out.view(-1, 8 * 8 * 8)
        out = self.act3(self.fc1(out))
        out = self.fc2(out)
        return out
```

This reshape is what we were missing earlier.

The `Net` class is equivalent to the `nn.Sequential` model we built earlier in terms of submodules; but by writing the `forward` function explicitly, we can manipulate the output of `self.pool3` directly and call `view` on it to turn it into a $B \times N$ vector. Note that we leave the batch dimension as –1 in the call to `view`, since in principle we don't know how many samples will be in the batch.

Here we use a subclass of `nn.Module` to contain our entire model. We could also use subclasses to define new building blocks for more complex networks. Picking up on the diagram style in chapter 6, our network looks like the one shown in figure 8.10. We are making some ad hoc choices about what information to present where.

Recall that the goal of classification networks typically is to compress information in the sense that we start with an image with a sizable number of pixels and compress it into (a vector of probabilities of) classes. Two things about our architecture deserve some commentary with respect to this goal.

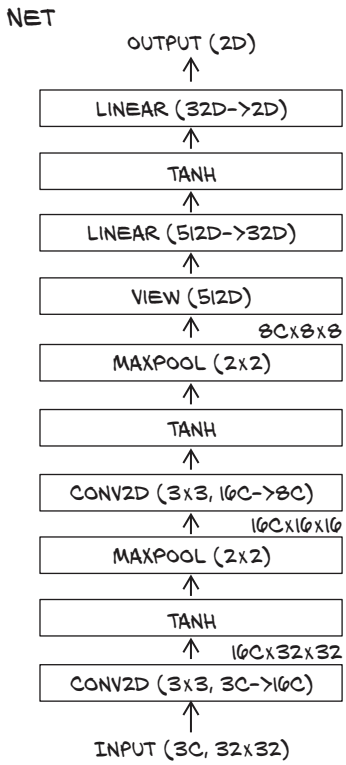


Figure 8.10 Our baseline convolutional network architecture

First, our goal is reflected by the size of our intermediate values generally shrinking—this is done by reducing the number of channels in the convolutions, by reducing the number of pixels through pooling, and by having an output dimension lower than the input dimension in the linear layers. This is a common trait of classification networks. However, in many popular architectures like the ResNets we saw in chapter 2 and discuss more in section 8.5.3, the reduction is achieved by pooling in the spatial resolution, but the number of channels increases (still resulting in a reduction in size). It seems that our pattern of fast information reduction works well with networks of limited depth and small images; but for deeper networks, the decrease is typically slower.

Second, in one layer, there is not a reduction of output size with regard to input size: the initial convolution. If we consider a single output pixel as a vector of 32 elements (the channels), it is a linear transformation of 27 elements (as a convolution of 3 channels × 3 × 3 kernel size)—only a moderate increase. In ResNet, the initial convolution generates 64 channels from 147 elements (3 channels × 7 × 7 kernel size).[6] So the first layer is exceptional in that it greatly increases the overall dimension (as in channels times pixels) of the data flowing through it, but the mapping for each output pixel considered in isolation still has approximately as many outputs as inputs.[7]

8.3.2 How PyTorch keeps track of parameters and submodules

Interestingly, assigning an instance of `nn.Module` to an attribute in an `nn.Module`, as we did in the earlier constructor, automatically registers the module as a submodule.

> **NOTE** The submodules must be top-level *attributes*, not buried inside `list` or `dict` instances! Otherwise the optimizer will not be able to locate the submodules (and, hence, their parameters). For situations where your model requires a list or dict of submodules, PyTorch provides `nn.ModuleList` and `nn.ModuleDict`.

We can call arbitrary methods of an `nn.Module` subclass. For example, for a model where training is substantially different than its use, say, for prediction, it may make sense to have a `predict` method. Be aware that calling such methods will be similar to calling `forward` instead of the module itself—they will be ignorant of hooks, and the JIT does not see the module structure when using them because we are missing the equivalent of the `__call__` bits shown in section 6.2.1.

This allows `Net` to have access to the parameters of its submodules without further action by the user:

---

[6] The dimensions in the pixel-wise linear mapping defined by the first convolution were emphasized by Jeremy Howard in his fast.ai course (https://www.fast.ai).

[7] Outside of and older than deep learning, projecting into high-dimensional space and then doing conceptually simpler (than linear) machine learning is commonly known as the *kernel trick*. The initial increase in the number of channels could be seen as a somewhat similar phenomenon, but striking a different balance between the cleverness of the embedding and the simplicity of the model working on the embedding.

```
# In[27]:
model = Net()

numel_list = [p.numel() for p in model.parameters()]
sum(numel_list), numel_list

# Out[27]:
(18090, [432, 16, 1152, 8, 16384, 32, 64, 2])
```

What happens here is that the `parameters()` call delves into all submodules assigned as attributes in the constructor and recursively calls `parameters()` on them. No matter how nested the submodule, any `nn.Module` can access the list of all child parameters. By accessing their `grad` attribute, which has been populated by `autograd`, the optimizer will know how to change parameters to minimize the loss. We know that story from chapter 5.

We now know how to implement our own modules—and we will need this a lot for part 2. Looking back at the implementation of the `Net` class, and thinking about the utility of registering submodules in the constructor so that we can access their parameters, it appears a bit of a waste that we are also registering submodules that have no parameters, like `nn.Tanh` and `nn.MaxPool2d`. Wouldn't it be easier to call these directly in the `forward` function, just as we called `view`?

8.3.3 The functional API

It sure would! And that's why PyTorch has *functional* counterparts for every `nn` module. By "functional" here we mean "having no internal state"—in other words, "whose output value is solely and fully determined by the value input arguments." Indeed, `torch.nn.functional` provides many functions that work like the modules we find in `nn`. But instead of working on the input arguments and stored parameters like the module counterparts, they take inputs and parameters as arguments to the function call. For instance, the functional counterpart of `nn.Linear` is `nn.functional.linear`, which is a function that has signature `linear(input, weight, bias=None)`. The `weight` and `bias` parameters are arguments to the function.

Back to our model, it makes sense to keep using `nn` modules for `nn.Linear` and `nn.Conv2d` so that `Net` will be able to manage their `Parameter`s during training. However, we can safely switch to the functional counterparts of pooling and activation, since they have no parameters:

```
# In[28]:
import torch.nn.functional as F

class Net(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(3, 16, kernel_size=3, padding=1)
        self.conv2 = nn.Conv2d(16, 8, kernel_size=3, padding=1)
        self.fc1 = nn.Linear(8 * 8 * 8, 32)
        self.fc2 = nn.Linear(32, 2)
```

```
    def forward(self, x):
        out = F.max_pool2d(torch.tanh(self.conv1(x)), 2)
        out = F.max_pool2d(torch.tanh(self.conv2(out)), 2)
        out = out.view(-1, 8 * 8 * 8)
        out = torch.tanh(self.fc1(out))
        out = self.fc2(out)
        return out
```

This is a lot more concise than and fully equivalent to our previous definition of `Net` in section 8.3.1. Note that it would still make sense to instantiate modules that require several parameters for their initialization in the constructor.

TIP While general-purpose scientific functions like `tanh` still exist in `torch.nn.functional` in version 1.0, those entry points are deprecated in favor of functions in the top-level `torch` namespace. More niche functions like `max_pool2d` will remain in `torch.nn.functional`.

Thus, the functional way also sheds light on what the `nn.Module` API is all about: a `Module` is a container for state in the forms of `Parameter`s and submodules combined with the instructions to do a forward.

Whether to use the functional or the modular API is a decision based on style and taste. When part of a network is so simple that we want to use `nn.Sequential`, we're in the modular realm. When we are writing our own forwards, it may be more natural to use the functional interface for things that do not need state in the form of parameters.

In chapter 15, we will briefly touch on quantization. Then stateless bits like activations suddenly become stateful because information about the quantization needs to be captured. This means if we aim to quantize our model, it might be worthwhile to stick with the modular API if we go for non-JITed quantization. There is one style matter that will help you avoid surprises with (originally unforeseen) uses: if you need several applications of stateless modules (like `nn.HardTanh` or `nn.ReLU`), it is probably a good idea to have a separate instance for each. Reusing the same module appears to be clever and will give correct results with our standard Python usage here, but tools analyzing your model may trip over it.

So now we can make our own `nn.Module` if we need to, and we also have the functional API for cases when instantiating and then calling an `nn.Module` is overkill. This has been the last bit missing to understand how the code organization works in just about any neural network implemented in PyTorch.

Let's double-check that our model runs, and then we'll get to the training loop:

```
# In[29]:
model = Net()
model(img.unsqueeze(0))

# Out[29]:
tensor([[-0.0157,  0.1143]], grad_fn=<AddmmBackward>)
```

We got two numbers! Information flows correctly. We might not realize it right now, but in more complex models, getting the size of the first linear layer right is sometimes a source of frustration. We've heard stories of famous practitioners putting in arbitrary numbers and then relying on error messages from PyTorch to backtrack the correct sizes for their linear layers. Lame, eh? Nah, it's all legit!

8.4 Training our convnet

We're now at the point where we can assemble our complete training loop. We already developed the overall structure in chapter 5, and the training loop looks much like the one from chapter 6, but here we will revisit it to add some details like some tracking for accuracy. After we run our model, we will also have an appetite for a little more speed, so we will learn how to run our models fast on a GPU. But first let's look at the training loop.

Recall that the core of our convnet is two nested loops: an outer one over the *epochs* and an inner one of the `DataLoader` that produces batches from our `Dataset`. In each loop, we then have to

1. Feed the inputs through the model (the forward pass).
2. Compute the loss (also part of the forward pass).
3. Zero any old gradients.
4. Call `loss.backward()` to compute the gradients of the loss with respect to all parameters (the backward pass).
5. Have the optimizer take a step in toward lower loss.

Also, we collect and print some information. So here is our training loop, looking almost as it does in the previous chapter—but it is good to remember what each thing is doing:

Uses the datetime module included with Python

```
# In[30]:
import datetime

def training_loop(n_epochs, optimizer, model, loss_fn, train_loader):
    for epoch in range(1, n_epochs + 1):
        loss_train = 0.0
        for imgs, labels in train_loader:

            outputs = model(imgs)

            loss = loss_fn(outputs, labels)

            optimizer.zero_grad()

            loss.backward()

            optimizer.step()
```

Our loop over the epochs, numbered from 1 to n_epochs rather than starting at 0

Loops over our dataset in the batches the data loader creates for us

Feeds a batch through our model …

… and computes the loss we wish to minimize

After getting rid of the gradients from the last round …

… performs the backward step. That is, we compute the gradients of all parameters we want the network to learn.

Updates the model

```
        loss_train += loss.item()

    if epoch == 1 or epoch % 10 == 0:
        print('{} Epoch {}, Training loss {}'.format(
            datetime.datetime.now(), epoch,
            loss_train / len(train_loader)))
```

Sums the losses we saw over the epoch. Recall that it is important to transform the loss to a Python number with .item(), to escape the gradients.

Divides by the length of the training data loader to get the average loss per batch. This is a much more intuitive measure than the sum.

We use the `Dataset` from chapter 7; wrap it into a `DataLoader`; instantiate our network, an optimizer, and a loss function as before; and call our training loop.

The substantial changes in our model from the last chapter are that now our model is a custom subclass of `nn.Module` and that we're using convolutions. Let's run training for 100 epochs while printing the loss. Depending on your hardware, this may take 20 minutes or more to finish!

The DataLoader batches up the examples of our cifar2 dataset. Shuffling randomizes the order of the examples from the dataset.

```
# In[31]:
train_loader = torch.utils.data.DataLoader(cifar2, batch_size=64,
                                           shuffle=True)

model = Net()  #
optimizer = optim.SGD(model.parameters(), lr=1e-2)  #
loss_fn = nn.CrossEntropyLoss()  #

training_loop(
    n_epochs = 100,
    optimizer = optimizer,
    model = model,
    loss_fn = loss_fn,
    train_loader = train_loader,
)

# Out[31]:
2020-01-16 23:07:21.889707 Epoch 1, Training loss 0.5634813266954605
2020-01-16 23:07:37.560610 Epoch 10, Training loss 0.3277610331109375
2020-01-16 23:07:54.966180 Epoch 20, Training loss 0.3035225479086493
2020-01-16 23:08:12.361597 Epoch 30, Training loss 0.28249378549824855
2020-01-16 23:08:29.769820 Epoch 40, Training loss 0.2611226033253275
2020-01-16 23:08:47.185401 Epoch 50, Training loss 0.24105800626574048
2020-01-16 23:09:04.644522 Epoch 60, Training loss 0.21997178820477928
2020-01-16 23:09:22.079625 Epoch 70, Training loss 0.20370126601047578
2020-01-16 23:09:39.593780 Epoch 80, Training loss 0.18939699422401987
2020-01-16 23:09:57.111441 Epoch 90, Training loss 0.17283396527266046
2020-01-16 23:10:14.632351 Epoch 100, Training loss 0.1614033816868712
```

Instantiates our network …

… the stochastic gradient descent optimizer we have been working with …

… and the cross entropy loss we met in 7.10

Calls the training loop we defined earlier

So now we can train our network. But again, our friend the bird watcher will likely not be impressed when we tell her that we trained to very low training loss.

8.4.1 Measuring accuracy

In order to have a measure that is more interpretable than the loss, we can take a look at our accuracies on the training and validation datasets. We use the same code as in chapter 7:

```
# In[32]:
train_loader = torch.utils.data.DataLoader(cifar2, batch_size=64,
                                           shuffle=False)
val_loader = torch.utils.data.DataLoader(cifar2_val, batch_size=64,
                                         shuffle=False)

def validate(model, train_loader, val_loader):
    for name, loader in [("train", train_loader), ("val", val_loader)]:
        correct = 0
        total = 0

        with torch.no_grad():
            for imgs, labels in loader:
                outputs = model(imgs)
                _, predicted = torch.max(outputs, dim=1)
                total += labels.shape[0]
                correct += int((predicted == labels).sum())

        print("Accuracy {}: {:.2f}".format(name , correct / total))

validate(model, train_loader, val_loader)

# Out[32]:
Accuracy train: 0.93
Accuracy val: 0.89
```

We do not want gradients here, as we will not want to update the parameters.

Counts the number of examples, so total is increased by the batch size

Gives us the index of the highest value as output

Comparing the predicted class that had the maximum probability and the ground-truth labels, we first get a Boolean array. Taking the sum gives the number of items in the batch where the prediction and ground truth agree.

We cast to a Python `int`—for integer tensors, this is equivalent to using `.item()`, similar to what we did in the training loop.

This is quite a lot better than the fully connected model, which achieved only 79% accuracy. We about halved the number of errors on the validation set. Also, we used far fewer parameters. This is telling us that the model does a better job of generalizing its task of recognizing the subject of images from a new sample, through locality and translation invariance. We could now let it run for more epochs and see what performance we could squeeze out.

8.4.2 Saving and loading our model

Since we're satisfied with our model so far, it would be nice to actually save it, right? It's easy to do. Let's save the model to a file:

```
# In[33]:
torch.save(model.state_dict(), data_path + 'birds_vs_airplanes.pt')
```

The birds_vs_airplanes.pt file now contains all the parameters of `model`: that is, weights and biases for the two convolution modules and the two linear modules. So,

no structure—just the weights. This means when we deploy the model in production for our friend, we'll need to keep the `model` class handy, create an instance, and then load the parameters back into it:

```
# In[34]:
loaded_model = Net()
loaded_model.load_state_dict(torch.load(data_path
                                        + 'birds_vs_airplanes.pt'))

# Out[34]:
<All keys matched successfully>
```

We will have to make sure we don't change the definition of Net between saving and later loading the model state.

We have also included a pretrained model in our code repository, saved to ../data/p1ch7/birds_vs_airplanes.pt.

8.4.3 Training on the GPU

We have a net and can train it! But it would be good to make it a bit faster. It is no surprise by now that we do so by moving our training onto the GPU. Using the `.to` method we saw in chapter 3, we can move the tensors we get from the data loader to the GPU, after which our computation will automatically take place there. But we also need to move our parameters to the GPU. Happily, `nn.Module` implements a `.to` function that moves all of its parameters to the GPU (or casts the type when you pass a `dtype` argument).

There is a somewhat subtle difference between `Module.to` and `Tensor.to`. `Module.to` is in place: the module instance is modified. But `Tensor.to` is out of place (in some ways computation, just like `Tensor.tanh`), returning a new tensor. One implication is that it is good practice to create the `Optimizer` after moving the parameters to the appropriate device.

It is considered good style to move things to the GPU if one is available. A good pattern is to set the a variable `device` depending on `torch.cuda.is_available`:

```
# In[35]:
device = (torch.device('cuda') if torch.cuda.is_available()
          else torch.device('cpu'))
print(f"Training on device {device}.")
```

Then we can amend the training loop by moving the tensors we get from the data loader to the GPU by using the `Tensor.to` method. Note that the code is exactly like our first version at the beginning of this section except for the two lines moving the inputs to the GPU:

```
# In[36]:
import datetime

def training_loop(n_epochs, optimizer, model, loss_fn, train_loader):
    for epoch in range(1, n_epochs + 1):
        loss_train = 0.0
```

```
        for imgs, labels in train_loader:
            imgs = imgs.to(device=device)
            labels = labels.to(device=device)
            outputs = model(imgs)
            loss = loss_fn(outputs, labels)

            optimizer.zero_grad()
            loss.backward()
            optimizer.step()

            loss_train += loss.item()

        if epoch == 1 or epoch % 10 == 0:
            print('{} Epoch {}, Training loss {}'.format(
                datetime.datetime.now(), epoch,
                loss_train / len(train_loader)))
```

These two lines that move imgs and labels to the device we are training on are the only difference from our previous version.

The same amendment must be made to the `validate` function. We can then instantiate our model, move it to `device`, and run it as before:[8]

```
# In[37]:
train_loader = torch.utils.data.DataLoader(cifar2, batch_size=64,
                                           shuffle=True)

model = Net().to(device=device)
optimizer = optim.SGD(model.parameters(), lr=1e-2)
loss_fn = nn.CrossEntropyLoss()

training_loop(
    n_epochs = 100,
    optimizer = optimizer,
    model = model,
    loss_fn = loss_fn,
    train_loader = train_loader,
)

# Out[37]:
2020-01-16 23:10:35.563216 Epoch 1, Training loss 0.5717791349265227
2020-01-16 23:10:39.730262 Epoch 10, Training loss 0.3285350770137872
2020-01-16 23:10:45.906321 Epoch 20, Training loss 0.29493294959994637
2020-01-16 23:10:52.086905 Epoch 30, Training loss 0.26962305994550134
2020-01-16 23:10:56.551582 Epoch 40, Training loss 0.24709946277794564
2020-01-16 23:11:00.991432 Epoch 50, Training loss 0.22623272664892446
2020-01-16 23:11:05.421524 Epoch 60, Training loss 0.20996672821462534
2020-01-16 23:11:09.951312 Epoch 70, Training loss 0.1934866009719053
2020-01-16 23:11:14.499484 Epoch 80, Training loss 0.1799132404908253
2020-01-16 23:11:19.047609 Epoch 90, Training loss 0.16620008706761774
2020-01-16 23:11:23.590435 Epoch 100, Training loss 0.15667157247662544
```

Moves our model (all parameters) to the GPU. If you forget to move either the model or the inputs to the GPU, you will get errors about tensors not being on the same device, because the PyTorch operators do not support mixing GPU and CPU inputs.

[8] There is a `pin_memory` option for the data loader that will cause the data loader to use memory pinned to the GPU, with the goal of speeding up transfers. Whether we gain something varies, though, so we will not pursue this here.

Even for our small network here, we do see a sizable increase in speed. The advantage of computing on GPUs is more visible for larger models.

There is a slight complication when loading network weights: PyTorch will attempt to load the weight to the same device it was saved from—that is, weights on the GPU will be restored to the GPU. As we don't know whether we want the same device, we have two options: we could move the network to the CPU before saving it, or move it back after restoring. It is a bit more concise to instruct PyTorch to override the device information when loading weights. This is done by passing the `map_location` keyword argument to `torch.load`:

```
# In[39]:
loaded_model = Net().to(device=device)
loaded_model.load_state_dict(torch.load(data_path
                                        + 'birds_vs_airplanes.pt',
                                        map_location=device))

# Out[39]:
<All keys matched successfully>
```

8.5 Model design

We built our model as a subclass of `nn.Module`, the de facto standard for all but the simplest models. Then we trained it successfully and saw how to use the GPU to train our models. We've reached the point where we can build a feed-forward convolutional neural network and train it successfully to classify images. The natural question is, what now? What if we are presented with a more complicated problem? Admittedly, our birds versus airplanes dataset wasn't that complicated: the images were very small, and the object under investigation was centered and took up most of the viewport.

If we moved to, say, ImageNet, we would find larger, more complex images, where the right answer would depend on multiple visual clues, often hierarchically organized. For instance, when trying to predict whether a dark brick shape is a remote control or a cell phone, the network could be looking for something like a screen.

Plus images may not be our sole focus in the real world, where we have tabular data, sequences, and text. The promise of neural networks is sufficient flexibility to solve problems on all these kinds of data given the proper architecture (that is, the interconnection of layers or modules) and the proper loss function.

PyTorch ships with a very comprehensive collection of modules and loss functions to implement state-of-the-art architectures ranging from feed-forward components to long short-term memory (LSTM) modules and transformer networks (two very popular architectures for sequential data). Several models are available through PyTorch Hub or as part of `torchvision` and other vertical community efforts.

We'll see a few more advanced architectures in part 2, where we'll walk through an end-to-end problem of analyzing CT scans, but in general, it is beyond the scope of this book to explore variations on neural network architectures. However, we can build on the knowledge we've accumulated thus far to understand how we can implement

almost any architecture thanks to the expressivity of PyTorch. The purpose of this section is precisely to provide conceptual tools that will allow us to read the latest research paper and start implementing it in PyTorch—or, since authors often release PyTorch implementations of their papers, to read the implementations without choking on our coffee.

8.5.1 Adding memory capacity: Width

Given our feed-forward architecture, there are a couple of dimensions we'd likely want to explore before getting into further complications. The first dimension is the *width* of the network: the number of neurons per layer, or channels per convolution. We can make a model wider very easily in PyTorch. We just specify a larger number of output channels in the first convolution and increase the subsequent layers accordingly, taking care to change the `forward` function to reflect the fact that we'll now have a longer vector once we switch to fully connected layers:

```
# In[40]:
class NetWidth(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(3, 32, kernel_size=3, padding=1)
        self.conv2 = nn.Conv2d(32, 16, kernel_size=3, padding=1)
        self.fc1 = nn.Linear(16 * 8 * 8, 32)
        self.fc2 = nn.Linear(32, 2)

    def forward(self, x):
        out = F.max_pool2d(torch.tanh(self.conv1(x)), 2)
        out = F.max_pool2d(torch.tanh(self.conv2(out)), 2)
        out = out.view(-1, 16 * 8 * 8)
        out = torch.tanh(self.fc1(out))
        out = self.fc2(out)
        return out
```

If we want to avoid hardcoding numbers in the definition of the model, we can easily pass a parameter to *init* and parameterize the width, taking care to also parameterize the call to `view` in the `forward` function:

```
# In[42]:
class NetWidth(nn.Module):
    def __init__(self, n_chans1=32):
        super().__init__()
        self.n_chans1 = n_chans1
        self.conv1 = nn.Conv2d(3, n_chans1, kernel_size=3, padding=1)
        self.conv2 = nn.Conv2d(n_chans1, n_chans1 // 2, kernel_size=3,
                               padding=1)
        self.fc1 = nn.Linear(8 * 8 * n_chans1 // 2, 32)
        self.fc2 = nn.Linear(32, 2)

    def forward(self, x):
        out = F.max_pool2d(torch.tanh(self.conv1(x)), 2)
        out = F.max_pool2d(torch.tanh(self.conv2(out)), 2)
```

```
        out = out.view(-1, 8 * 8 * self.n_chans1 // 2)
        out = torch.tanh(self.fc1(out))
        out = self.fc2(out)
        return out
```

The numbers specifying channels and features for each layer are directly related to the number of parameters in a model; all other things being equal, they increase the *capacity* of the model. As we did previously, we can look at how many parameters our model has now:

```
# In[44]:
sum(p.numel() for p in model.parameters())

# Out[44]:
38386
```

The greater the capacity, the more variability in the inputs the model will be able to manage; but at the same time, the more likely overfitting will be, since the model can use a greater number of parameters to memorize unessential aspects of the input. We already went into ways to combat overfitting, the best being increasing the sample size or, in the absence of new data, augmenting existing data through artificial modifications of the same data.

There are a few more tricks we can play at the model level (without acting on the data) to control overfitting. Let's review the most common ones.

8.5.2 Helping our model to converge and generalize: Regularization

Training a model involves two critical steps: optimization, when we need the loss to decrease on the training set; and generalization, when the model has to work not only on the training set but also on data it has not seen before, like the validation set. The mathematical tools aimed at easing these two steps are sometimes subsumed under the label *regularization*.

Keeping the parameters in check: Weight penalties

The first way to stabilize generalization is to add a regularization term to the loss. This term is crafted so that the weights of the model tend to be small on their own, limiting how much training makes them grow. In other words, it is a penalty on larger weight values. This makes the loss have a smoother topography, and there's relatively less to gain from fitting individual samples.

The most popular regularization terms of this kind are L2 regularization, which is the sum of squares of all weights in the model, and L1 regularization, which is the sum of the absolute values of all weights in the model.[9] Both of them are scaled by a (small) factor, which is a hyperparameter we set prior to training.

[9] We'll focus on L2 regularization here. L1 regularization—popularized in the more general statistics literature by its use in Lasso—has the attractive property of resulting in sparse trained weights.

L2 regularization is also referred to as *weight decay*. The reason for this name is that, thinking about SGD and backpropagation, the negative gradient of the L2 regularization term with respect to a parameter `w_i` is `- 2 * lambda * w_i`, where `lambda` is the aforementioned hyperparameter, simply named *weight decay* in PyTorch. So, adding L2 regularization to the loss function is equivalent to decreasing each weight by an amount proportional to its current value during the optimization step (hence, the name *weight decay*). Note that weight decay applies to all parameters of the network, such as biases.

In PyTorch, we could implement regularization pretty easily by adding a term to the loss. After computing the loss, whatever the loss function is, we can iterate the parameters of the model, sum their respective square (for L2) or `abs` (for L1), and backpropagate:

```
# In[45]:
def training_loop_l2reg(n_epochs, optimizer, model, loss_fn,
                        train_loader):
    for epoch in range(1, n_epochs + 1):
        loss_train = 0.0
        for imgs, labels in train_loader:
            imgs = imgs.to(device=device)
            labels = labels.to(device=device)
            outputs = model(imgs)
            loss = loss_fn(outputs, labels)

            l2_lambda = 0.001
            l2_norm = sum(p.pow(2.0).sum()
                          for p in model.parameters())
            loss = loss + l2_lambda * l2_norm

            optimizer.zero_grad()
            loss.backward()
            optimizer.step()

            loss_train += loss.item()
        if epoch == 1 or epoch % 10 == 0:
            print('{} Epoch {}, Training loss {}'.format(
                datetime.datetime.now(), epoch,
                loss_train / len(train_loader)))
```

Replaces pow(2.0) with abs() for L1 regularization

However, the SGD optimizer in PyTorch already has a `weight_decay` parameter that corresponds to `2 * lambda`, and it directly performs weight decay during the update as described previously. It is fully equivalent to adding the L2 norm of weights to the loss, without the need for accumulating terms in the loss and involving autograd.

NOT RELYING TOO MUCH ON A SINGLE INPUT: DROPOUT

An effective strategy for combating overfitting was originally proposed in 2014 by Nitish Srivastava and coauthors from Geoff Hinton's group in Toronto, in a paper aptly entitled "Dropout: a Simple Way to Prevent Neural Networks from Overfitting" (http://mng.bz/nPMa). Sounds like pretty much exactly what we're looking for,

right? The idea behind dropout is indeed simple: zero out a random fraction of outputs from neurons across the network, where the randomization happens at each training iteration.

This procedure effectively generates slightly different models with different neuron topologies at each iteration, giving neurons in the model less chance to coordinate in the memorization process that happens during overfitting. An alternative point of view is that dropout perturbs the features being generated by the model, exerting an effect that is close to augmentation, but this time throughout the network.

In PyTorch, we can implement dropout in a model by adding an `nn.Dropout` module between the nonlinear activation function and the linear or convolutional module of the subsequent layer. As an argument, we need to specify the probability with which inputs will be zeroed out. In case of convolutions, we'll use the specialized `nn.Dropout2d` or `nn.Dropout3d`, which zero out entire channels of the input:

```
# In[47]:
class NetDropout(nn.Module):
    def __init__(self, n_chans1=32):
        super().__init__()
        self.n_chans1 = n_chans1
        self.conv1 = nn.Conv2d(3, n_chans1, kernel_size=3, padding=1)
        self.conv1_dropout = nn.Dropout2d(p=0.4)
        self.conv2 = nn.Conv2d(n_chans1, n_chans1 // 2, kernel_size=3,
                               padding=1)
        self.conv2_dropout = nn.Dropout2d(p=0.4)
        self.fc1 = nn.Linear(8 * 8 * n_chans1 // 2, 32)
        self.fc2 = nn.Linear(32, 2)

    def forward(self, x):
        out = F.max_pool2d(torch.tanh(self.conv1(x)), 2)
        out = self.conv1_dropout(out)
        out = F.max_pool2d(torch.tanh(self.conv2(out)), 2)
        out = self.conv2_dropout(out)
        out = out.view(-1, 8 * 8 * self.n_chans1 // 2)
        out = torch.tanh(self.fc1(out))
        out = self.fc2(out)
        return out
```

Note that dropout is normally active during training, while during the evaluation of a trained model in production, dropout is bypassed or, equivalently, assigned a probability equal to zero. This is controlled through the `train` property of the `Dropout` module. Recall that PyTorch lets us switch between the two modalities by calling

```
model.train()
```

or

```
model.eval()
```

on any `nn.Model` subclass. The call will be automatically replicated on the submodules so that if `Dropout` is among them, it will behave accordingly in subsequent forward and backward passes.

KEEPING ACTIVATIONS IN CHECK: BATCH NORMALIZATION

Dropout was all the rage when, in 2015, another seminal paper was published by Sergey Ioffe and Christian Szegedy from Google, entitled "Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift" (https://arxiv.org/abs/1502.03167). The paper described a technique that had multiple beneficial effects on training: allowing us to increase the learning rate and make training less dependent on initialization and act as a regularizer, thus representing an alternative to dropout.

The main idea behind batch normalization is to rescale the inputs to the activations of the network so that minibatches have a certain desirable distribution. Recalling the mechanics of learning and the role of nonlinear activation functions, this helps avoid the inputs to activation functions being too far into the saturated portion of the function, thereby killing gradients and slowing training.

In practical terms, batch normalization shifts and scales an intermediate input using the mean and standard deviation collected at that intermediate location over the samples of the minibatch. The regularization effect is a result of the fact that an individual sample and its downstream activations are always seen by the model as shifted and scaled, depending on the statistics across the randomly extracted minibatch. This is in itself a form of *principled* augmentation. The authors of the paper suggest that using batch normalization eliminates or at least alleviates the need for dropout.

Batch normalization in PyTorch is provided through the `nn.BatchNorm1D`, `nn.BatchNorm2d`, and `nn.BatchNorm3d` modules, depending on the dimensionality of the input. Since the aim for batch normalization is to rescale the inputs of the activations, the natural location is after the linear transformation (convolution, in this case) and the activation, as shown here:

```
# In[49]:
class NetBatchNorm(nn.Module):
    def __init__(self, n_chans1=32):
        super().__init__()
        self.n_chans1 = n_chans1
        self.conv1 = nn.Conv2d(3, n_chans1, kernel_size=3, padding=1)
        self.conv1_batchnorm = nn.BatchNorm2d(num_features=n_chans1)
        self.conv2 = nn.Conv2d(n_chans1, n_chans1 // 2, kernel_size=3,
                               padding=1)
        self.conv2_batchnorm = nn.BatchNorm2d(num_features=n_chans1 // 2)
        self.fc1 = nn.Linear(8 * 8 * n_chans1 // 2, 32)
        self.fc2 = nn.Linear(32, 2)

    def forward(self, x):
        out = self.conv1_batchnorm(self.conv1(x))
        out = F.max_pool2d(torch.tanh(out), 2)
```

```
        out = self.conv2_batchnorm(self.conv2(out))
        out = F.max_pool2d(torch.tanh(out), 2)
        out = out.view(-1, 8 * 8 * self.n_chans1 // 2)
        out = torch.tanh(self.fc1(out))
        out = self.fc2(out)
        return out
```

Just as for dropout, batch normalization needs to behave differently during training and inference. In fact, at inference time, we want to avoid having the output for a specific input depend on the statistics of the other inputs we're presenting to the model. As such, we need a way to still normalize, but this time fixing the normalization parameters once and for all.

As minibatches are processed, in addition to estimating the mean and standard deviation for the current minibatch, PyTorch also updates the running estimates for mean and standard deviation that are representative of the whole dataset, as an approximation. This way, when the user specifies

```
model.eval()
```

and the model contains a batch normalization module, the running estimates are frozen and used for normalization. To unfreeze running estimates and return to using the minibatch statistics, we call `model.train()`, just as we did for dropout.

8.5.3 Going deeper to learn more complex structures: Depth

Earlier, we talked about width as the first dimension to act on in order to make a model larger and, in a way, more capable. The second fundamental dimension is obviously *depth*. Since this is a deep learning book, depth is something we're supposedly into. After all, deeper models are always better than shallow ones, aren't they? Well, it depends. With depth, the complexity of the function the network is able to approximate generally increases. In regard to computer vision, a shallower network could identify a person's shape in a photo, whereas a deeper network could identify the person, the face on their top half, and the mouth within the face. Depth allows a model to deal with hierarchical information when we need to understand the context in order to say something about some input.

There's another way to think about depth: increasing depth is related to increasing the length of the sequence of operations that the network will be able to perform when processing input. This view—of a deep network that performs sequential operations to carry out a task—is likely fascinating to software developers who are used to thinking about algorithms as sequences of operations like "find the person's boundaries, look for the head on top of the boundaries, look for the mouth within the head."

Skip connections

Depth comes with some additional challenges, which prevented deep learning models from reaching 20 or more layers until late 2015. Adding depth to a model generally makes training harder to converge. Let's recall backpropagation and think about it in

the context of a very deep network. The derivatives of the loss function with respect to the parameters, especially those in early layers, need to be multiplied by a lot of other numbers originating from the chain of derivative operations between the loss and the parameter. Those numbers being multiplied could be small, generating ever-smaller numbers, or large, swallowing smaller numbers due to floating-point approximation. The bottom line is that a long chain of multiplications will tend to make the contribution of the parameter to the gradient *vanish*, leading to ineffective training of that layer since that parameter and others like it won't be properly updated.

In December 2015, Kaiming He and coauthors presented *residual networks* (ResNets), an architecture that uses a simple trick to allow very deep networks to be successfully trained (https://arxiv.org/abs/1512.03385). That work opened the door to networks ranging from tens of layers to 100 layers in depth, surpassing the then state of the art in computer vision benchmark problems. We encountered residual networks when we were playing with pretrained models in chapter 2. The trick we mentioned is the following: using a *skip connection* to short-circuit blocks of layers, as shown in figure 8.11.

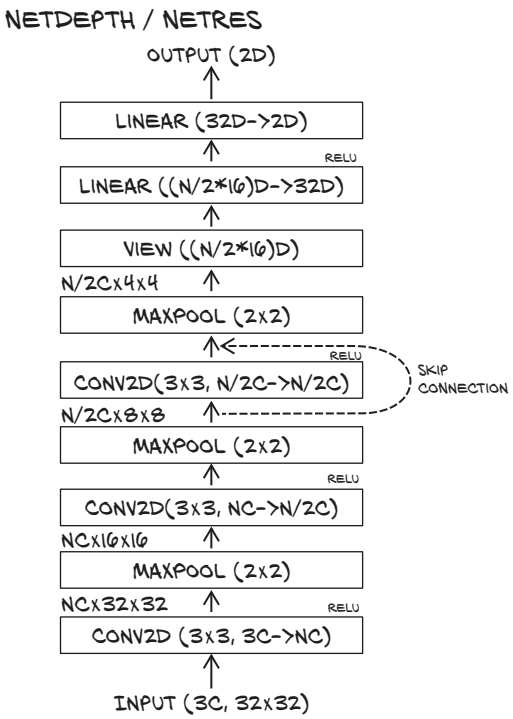


Figure 8.11 The architecture of our network with three convolutional layers. The skip connection is what differentiates `NetRes` from `NetDepth`.

A skip connection is nothing but the addition of the input to the output of a block of layers. This is exactly how it is done in PyTorch. Let's add one layer to our simple convolutional model, and let's use ReLU as the activation for a change. The vanilla module with an extra layer looks like this:

```
# In[51]:
class NetDepth(nn.Module):
    def __init__(self, n_chans1=32):
        super().__init__()
        self.n_chans1 = n_chans1
        self.conv1 = nn.Conv2d(3, n_chans1, kernel_size=3, padding=1)
        self.conv2 = nn.Conv2d(n_chans1, n_chans1 // 2, kernel_size=3,
                               padding=1)
        self.conv3 = nn.Conv2d(n_chans1 // 2, n_chans1 // 2,
                               kernel_size=3, padding=1)
        self.fc1 = nn.Linear(4 * 4 * n_chans1 // 2, 32)
        self.fc2 = nn.Linear(32, 2)
```

```
    def forward(self, x):
        out = F.max_pool2d(torch.relu(self.conv1(x)), 2)
        out = F.max_pool2d(torch.relu(self.conv2(out)), 2)
        out = F.max_pool2d(torch.relu(self.conv3(out)), 2)
        out = out.view(-1, 4 * 4 * self.n_chans1 // 2)
        out = torch.relu(self.fc1(out))
        out = self.fc2(out)
        return out
```

Adding a skip connection a la ResNet to this model amounts to adding the output of the first layer in the `forward` function to the input of the third layer:

```
# In[53]:
class NetRes(nn.Module):
    def __init__(self, n_chans1=32):
        super().__init__()
        self.n_chans1 = n_chans1
        self.conv1 = nn.Conv2d(3, n_chans1, kernel_size=3, padding=1)
        self.conv2 = nn.Conv2d(n_chans1, n_chans1 // 2, kernel_size=3,
                               padding=1)
        self.conv3 = nn.Conv2d(n_chans1 // 2, n_chans1 // 2,
                               kernel_size=3, padding=1)
        self.fc1 = nn.Linear(4 * 4 * n_chans1 // 2, 32)
        self.fc2 = nn.Linear(32, 2)

    def forward(self, x):
        out = F.max_pool2d(torch.relu(self.conv1(x)), 2)
        out = F.max_pool2d(torch.relu(self.conv2(out)), 2)
        out1 = out
        out = F.max_pool2d(torch.relu(self.conv3(out)) + out1, 2)
        out = out.view(-1, 4 * 4 * self.n_chans1 // 2)
        out = torch.relu(self.fc1(out))
        out = self.fc2(out)
        return out
```

In other words, we're using the output of the first activations as inputs to the last, in addition to the standard feed-forward path. This is also referred to as *identity mapping*. So, how does this alleviate the issues with vanishing gradients we were mentioning earlier?

Thinking about backpropagation, we can appreciate that a skip connection, or a sequence of skip connections in a deep network, creates a direct path from the deeper parameters to the loss. This makes their contribution to the gradient of the loss more direct, as partial derivatives of the loss with respect to those parameters have a chance not to be multiplied by a long chain of other operations.

It has been observed that skip connections have a beneficial effect on convergence especially in the initial phases of training. Also, the loss landscape of deep residual networks is a lot smoother than feed-forward networks of the same depth and width.

It is worth noting that skip connections were not new to the world when ResNets came along. Highway networks and U-Net made use of skip connections of one form

or another. However, the way ResNets used skip connections enabled models of depths greater than 100 to be amenable to training.

Since the advent of ResNets, other architectures have taken skip connections to the next level. One in particular, DenseNet, proposed to connect each layer with several other layers downstream through skip connections, achieving state-of-the-art results with fewer parameters. By now, we know how to implement something like DenseNets: just arithmetically add earlier intermediate outputs to downstream intermediate outputs.

BUILDING VERY DEEP MODELS IN PYTORCH

We talked about exceeding 100 layers in a convolutional neural network. How can we build that network in PyTorch without losing our minds in the process? The standard strategy is to define a building block, such as a `(Conv2d, ReLU, Conv2d) + skip connection` block, and then build the network dynamically in a `for` loop. Let's see it done in practice. We will create the network depicted in figure 8.12.

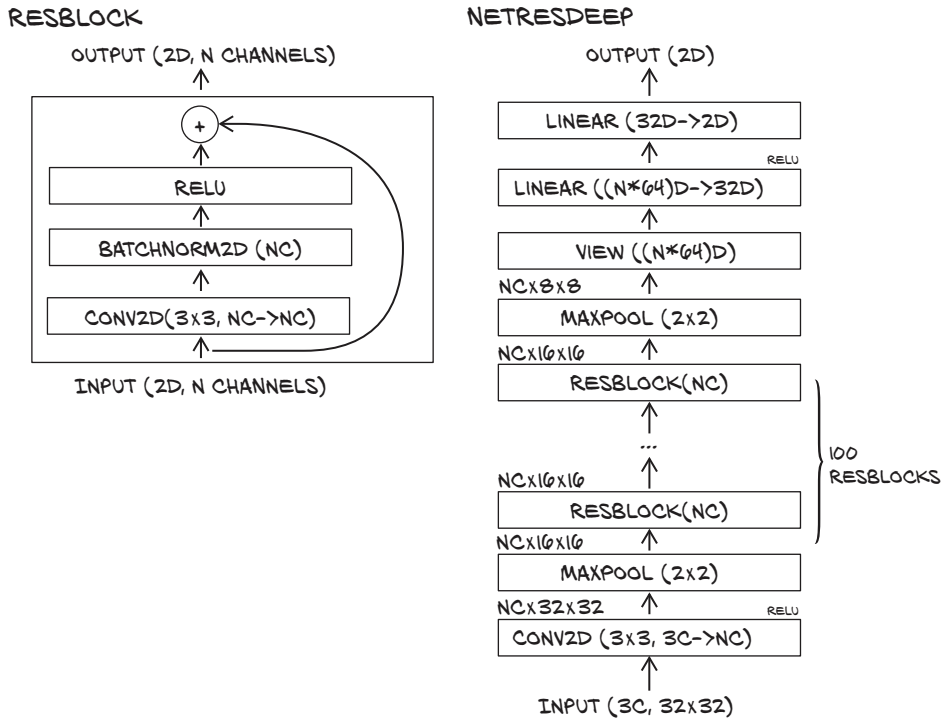


Figure 8.12 Our deep architecture with residual connections. On the left, we define a simplistic residual block. We use it as a building block in our network, as shown on the right.

We first create a module subclass whose sole job is to provide the computation for one *block*—that is, one group of convolutions, activation, and skip connection:

```
# In[55]:
class ResBlock(nn.Module):
    def __init__(self, n_chans):
        super(ResBlock, self).__init__()
        self.conv = nn.Conv2d(n_chans, n_chans, kernel_size=3,
                              padding=1, bias=False)
        self.batch_norm = nn.BatchNorm2d(num_features=n_chans)
        torch.nn.init.kaiming_normal_(self.conv.weight,
                                      nonlinearity='relu')
        torch.nn.init.constant_(self.batch_norm.weight, 0.5)
        torch.nn.init.zeros_(self.batch_norm.bias)

    def forward(self, x):
        out = self.conv(x)
        out = self.batch_norm(out)
        out = torch.relu(out)
        return out + x
```

The BatchNorm layer would cancel the effect of bias, so it is customarily left out.

Uses custom initializations . kaiming_normal_ initializes with normal random elements with standard deviation as computed in the ResNet paper. The batch norm is initialized to produce output distributions that initially have 0 mean and 0.5 variance.

Since we're planning to generate a deep model, we are including batch normalization in the block, since this will help prevent gradients from vanishing during training. We'd now like to generate a 100-block network. Does this mean we have to prepare for some serious cutting and pasting? Not at all; we already have the ingredients for imagining how this could look like.

First, in *init*, we create `nn.Sequential` containing a list of `ResBlock` instances. `nn.Sequential` will ensure that the output of one block is used as input to the next. It will also ensure that all the parameters in the block are visible to `Net`. Then, in `forward`, we just call the sequential to traverse the 100 blocks and generate the output:

```
# In[56]:
class NetResDeep(nn.Module):
    def __init__(self, n_chans1=32, n_blocks=10):
        super().__init__()
        self.n_chans1 = n_chans1
        self.conv1 = nn.Conv2d(3, n_chans1, kernel_size=3, padding=1)
        self.resblocks = nn.Sequential(
            *(n_blocks * [ResBlock(n_chans=n_chans1)]))
        self.fc1 = nn.Linear(8 * 8 * n_chans1, 32)
        self.fc2 = nn.Linear(32, 2)

    def forward(self, x):
        out = F.max_pool2d(torch.relu(self.conv1(x)), 2)
        out = self.resblocks(out)
        out = F.max_pool2d(out, 2)
        out = out.view(-1, 8 * 8 * self.n_chans1)
        out = torch.relu(self.fc1(out))
        out = self.fc2(out)
        return out
```

In the implementation, we parameterize the actual number of layers, which is important for experimentation and reuse. Also, needless to say, backpropagation will work as expected. Unsurprisingly, the network is quite a bit slower to converge. It is also more

fragile in convergence. This is why we used more-detailed initializations and trained our `NetRes` with a learning rate of 3e – 3 instead of the 1e – 2 we used for the other networks. We trained none of the networks to convergence, but we would not have gotten anywhere without these tweaks.

All this shouldn't encourage us to seek depth on a dataset of 32 × 32 images, but it clearly demonstrates how this can be achieved on more challenging datasets like ImageNet. It also provides the key elements for understanding existing implementations for models like ResNet, for instance, in `torchvision`.

INITIALIZATION

Let's briefly comment about the earlier initialization. Initialization is one of the important tricks in training neural networks. Unfortunately, for historical reasons, PyTorch has default weight initializations that are not ideal. People are looking at fixing the situation; if progress is made, it can be tracked on GitHub (https://github.com/pytorch/pytorch/issues/18182). In the meantime, we need to fix the weight initialization ourselves. We found that our model did not converge and looked at what people commonly choose as initialization (a smaller variance in weights; and zero mean and unit variance outputs for batch norm), and then we halved the output variance in the batch norm when the network would not converge.

Weight initialization could fill an entire chapter on its own, but we think that would be excessive. In chapter 11, we'll bump into initialization again and use what arguably could be PyTorch defaults without much explanation. Once you've progressed to the point where the details of weight initialization are of specific interest to you—probably not before finishing this book—you might revisit this topic.[10]

8.5.4 Comparing the designs from this section

We summarize the effect of each of our design modifications in isolation in figure 8.13. We should not overinterpret any of the specific numbers—our problem setup and experiments are simplistic, and repeating the experiment with different random seeds will probably generate variation at least as large as the differences in validation accuracy. For this demonstration, we left all other things equal, from learning rate to number of epochs to train; in practice, we would try to get the best results by varying those. Also, we would likely want to combine some of the additional design elements.

But a qualitative observation may be in order: as we saw in section 5.5.3, when discussing validatioin and overfitting, The weight decay and dropout regularizations, which have a more rigorous statistical estimation interpretation as regularization than batch norm, have a much narrower gap between the two accuracies. Batch norm, which

[10] The seminal paper on the topic is by X. Glorot and Y. Bengio: "Understanding the Difficulty of Training Deep Feedforward Neural Networks" (2010), which introduces PyTorch's *Xavier* initializations (http://mng.bz/vxz7). The ResNet paper we mentioned expands on the topic, too, giving us the Kaiming initializations used earlier. More recently, H. Zhang et al. have tweaked initialization to the point that they do not need batch norm in their experiments with very deep residual networks (https://arxiv.org/abs/1901.09321).

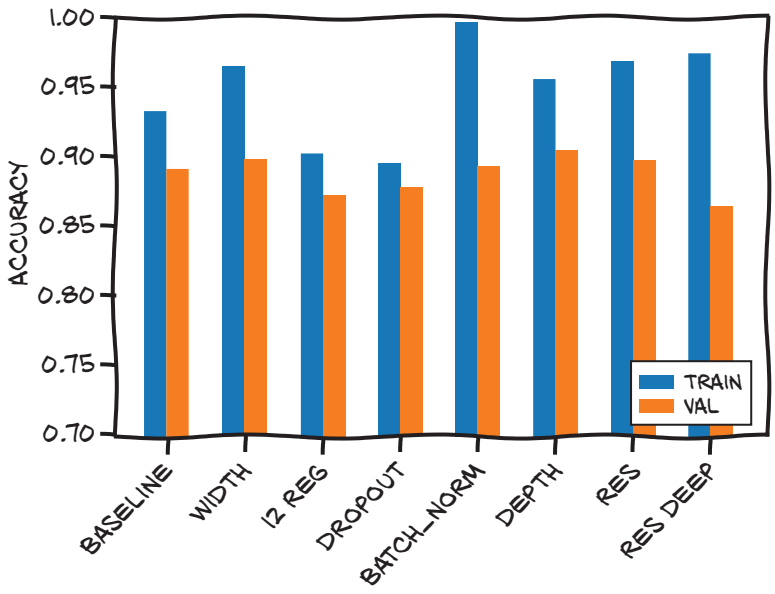


Figure 8.13 The modified networks all perform similarly.

serves more as a convergence helper, lets us train the network to nearly 100% training accuracy, so we interpret the first two as regularization.

8.5.5 It's already outdated

The curse and blessing of a deep learning practitioner is that neural network architectures evolve at a very rapid pace. This is not to say that what we've seen in this chapter is necessarily old school, but a thorough illustration of the latest and greatest architectures is a matter for another book (and they would cease to be the latest and the greatest pretty quickly anyway). The take-home message is that we should make every effort to proficiently translate the math behind a paper into actual PyTorch code, or at least understand the code that others have written with the same intention. In the last few chapters, you have hopefully gathered quite a few of the fundamental skills to translate ideas into implemented models in PyTorch.

8.6 Conclusion

After quite a lot of work, we now have a model that our fictional friend Jane can use to filter images for her blog. All we have to do is take an incoming image, crop and resize it to 32 × 32, and see what the model has to say about it. Admittedly, we have solved only part of the problem, but it was a journey in itself.

We have solved just part of the problem because there are a few interesting unknowns we would still have to face. One is picking out a bird or airplane from a

larger image. Creating bounding boxes around objects in an image is something a model like ours can't do.

Another hurdle concerns what happens when Fred the cat walks in front of the camera. Our model will not refrain from giving its opinion about how bird-like the cat is! It will happily output "airplane" or "bird," perhaps with 0.99 probability. This issue of being very confident about samples that are far from the training distribution is called *overgeneralization*. It's one of the main problems when we take a (presumably good) model to production in those cases where we can't really trust the input (which, sadly, is the majority of real-world cases).

In this chapter, we have built reasonable, working models in PyTorch that can learn from images. We did it in a way that helped us build our intuition around convolutional networks. We also explored ways in which we can make our models wider and deeper, while controlling effects like overfitting. Although we still only scratched the surface, we have taken another significant step ahead from the previous chapter. We now have a solid basis for facing the challenges we'll encounter when working on deep learning projects.

Now that we're familiar with PyTorch conventions and common features, we're ready to tackle something bigger. We're going to transition from a mode where each chapter or two presents a small problem, to spending multiple chapters breaking down a bigger, real-world problem. Part 2 uses automatic detection of lung cancer as an ongoing example; we will go from being familiar with the PyTorch API to being able to implement entire projects using PyTorch. We'll start in the next chapter by explaining the problem from a high level, and then we'll get into the details of the data we'll be using.

8.7 Exercises

1. Change our model to use a 5 × 5 kernel with `kernel_size=5` passed to the `nn.Conv2d` constructor.
   a. What impact does this change have on the number of parameters in the model?
   b. Does the change improve or degrade overfitting?
   c. Read https://pytorch.org/docs/stable/nn.html#conv2d.
   d. Can you describe what `kernel_size=(1,3)` will do?
   e. How does the model behave with such a kernel?
2. Can you find an image that contains neither a bird nor an airplane, but that the model claims has one or the other with more than 95% confidence?
   a. Can you manually edit a neutral image to make it more airplane-like?
   b. Can you manually edit an airplane image to trick the model into reporting a bird?
   c. Do these tasks get easier with a network with less capacity? More capacity?

8.8 Summary

- Convolution can be used as the linear operation of a feed-forward network dealing with images. Using convolution produces networks with fewer parameters, exploiting locality and featuring translation invariance.
- Stacking multiple convolutions with their activations one after the other, and using max pooling in between, has the effect of applying convolutions to increasingly smaller feature images, thereby effectively accounting for spatial relationships across larger portions of the input image as depth increases.
- Any `nn.Module` subclass can recursively collect and return its and its children's parameters. This technique can be used to count them, feed them into the optimizer, or inspect their values.
- The functional API provides modules that do not depend on storing internal state. It is used for operations that do not hold parameters and, hence, are not trained.
- Once trained, parameters of a model can be saved to disk and loaded back in with one line of code each.