

Dive into Deep Learning

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Preface

Just a few years ago, there were no legions of deep learning scientists developing intelligent products and services at major companies and startups. When we entered the field, machine learning did not command headlines in daily newspapers. Our parents had no idea what machine learning was, let alone why we might prefer it to a career in medicine or law. Machine learning was a blue skies academic discipline whose industrial significance was limited to a narrow set of real-world applications, including speech recognition and computer vision. Moreover, many of these applications required so much domain knowledge that they were often regarded as entirely separate areas for which machine learning was one small component. At that time, neural networks—the predecessors of the deep learning methods that we focus on in this book—were generally regarded as outmoded.

In just the past five years, deep learning has taken the world by surprise, driving rapid progress in such diverse fields as diverse as computer vision, natural language processing, automatic speech recognition, reinforcement learning, biomedical informatics, and has even catalyzed developments in theoretical machine learning and statistics. With these advances in hand, we can now build cars that drive themselves with more autonomy than ever before (and less autonomy than some companies might have you believe), smart reply systems that automatically draft the most mundane emails, helping people dig out from oppressively large inboxes, and software agents that dominate the world's best humans at board games like Go, a feat once thought to be decades away. Already, these tools exert ever-wider impacts on industry and society, changing the way movies are made, diseases are diagnosed, and playing a growing role in basic sciences—from astrophysics to biology.

About This Book

This book represents our attempt to make deep learning approachable, teaching you the *concepts*, the *context*, and the *code*.

One Medium Combining Code, Math, and HTML

For any computing technology to reach its full impact, it must be well-understood, well-documented, and supported by mature, well-maintained tools. The key ideas should be clearly distilled, minimizing the onboarding time needing to bring new practitioners up to date. Mature libraries should automate common tasks, and exemplar code should make it easy for practitioners to modify, apply, and extend common applications to suit their needs. Take dynamic web applications as an example. Despite a large number of companies, like Amazon, developing successful database-driven web applications in the 1990s, the potential of this technology to aid creative en-

trepreneurs has been realized to a far greater degree in the past ten years, owing in part to the development of powerful, well-documented frameworks.

Testing the potential of deep learning presents unique challenges because any single application brings together various disciplines. Applying deep learning requires simultaneously understanding (i) the motivations for casting a problem in a particular way; (ii) the mathematical form of a given model; (iii) the optimization algorithms for fitting the models to data; (iv) the basic statistical principles and intuitions that help us to extract generalizable insights from data; and (v) the engineering required to train models efficiently, navigating the pitfalls of numerical computing and getting the most out of available hardware. Teaching both the critical thinking skills required to formulate problems, the mathematics to solve them, and the software tools to implement those solutions all in one place presents formidable challenges. Our goal in this book is to present a unified resource to bring would-be practitioners up to speed.

When we started this book project, there were no resources that simultaneously (i) were up to date; (ii) covered the full breadth of modern machine learning with substantial technical depth; and (iii) interleaved exposition of the quality one expects from an engaging textbook with the clean runnable code that one expects to find in hands-on tutorials. We found plenty of code examples for how to use a given deep learning framework (e.g., how to do basic numerical computing with matrices in TensorFlow) or for implementing particular techniques (e.g., code snippets for LeNet, AlexNet, ResNets, etc) scattered across various blog posts and GitHub repositories. However, these examples typically focused on *how* to implement a given approach, but left out the discussion of *why* certain algorithmic decisions are made. While some interactive resources have popped up sporadically to address a particular topic, e.g., the engaging blog posts published on the website [Distill³](#), or personal blogs, they only covered selected topics in deep learning, and often lacked associated code. On the other hand, while several deep learning textbooks have emerged—e.g., ([Goodfellow et al., 2016](#)), which offers a comprehensive survey of the concepts behind deep learning—these resources do not marry the descriptions to realizations of the concepts in code, sometimes leaving readers clueless as to how to implement them. Moreover, too many resources are hidden behind the paywalls of commercial course providers.

We set out to create a resource that could (i) be freely available for everyone; (ii) offer sufficient technical depth to provide a starting point on the path to actually becoming an applied machine learning scientist; (iii) include runnable code, showing readers *how* to solve problems in practice; (iv) allow for rapid updates, both by us and also by the community at large; and (v) be complemented by a [forum⁴](#) for interactive discussion of technical details and to answer questions.

These goals were often in conflict. Equations, theorems, and citations are best managed and laid out in LaTeX. Code is best described in Python. And webpages are native in HTML and JavaScript. Furthermore, we want the content to be accessible both as executable code, as a physical book, as a downloadable PDF, and on the Internet as a website. At present there exist no tools and no workflow perfectly suited to these demands, so we had to assemble our own. We describe our approach in detail in [Section 19.6](#). We settled on GitHub to share the source and to facilitate community contributions, Jupyter notebooks for mixing code, equations and text, Sphinx as a rendering engine to generate multiple outputs, and Discourse for the forum. While our system is not yet perfect, these choices provide a good compromise among the competing concerns. We believe that this might be the first book published using such an integrated workflow.

³ <http://distill.pub>

⁴ <http://discuss.d2l.ai>

Learning by Doing

Many textbooks present concepts in succession, covering each in exhaustive detail. For example, Chris Bishop's excellent textbook ([Bishop, 2006](#)), teaches each topic so thoroughly that getting to the chapter on linear regression requires a non-trivial amount of work. While experts love this book precisely for its thoroughness, for true beginners, this property limits its usefulness as an introductory text.

In this book, we will teach most concepts *just in time*. In other words, you will learn concepts at the very moment that they are needed to accomplish some practical end. While we take some time at the outset to teach fundamental preliminaries, like linear algebra and probability, we want you to taste the satisfaction of training your first model before worrying about more esoteric probability distributions.

Aside from a few preliminary notebooks that provide a crash course in the basic mathematical background, each subsequent chapter introduces both a reasonable number of new concepts and provides single self-contained working examples—using real datasets. This presents an organizational challenge. Some models might logically be grouped together in a single notebook. And some ideas might be best taught by executing several models in succession. On the other hand, there is a big advantage to adhering to a policy of *one working example, one notebook*: This makes it as easy as possible for you to start your own research projects by leveraging our code. Just copy a notebook and start modifying it.

We will interleave the runnable code with background material as needed. In general, we will often err on the side of making tools available before explaining them fully (and we will follow up by explaining the background later). For instance, we might use *stochastic gradient descent* before fully explaining why it is useful or why it works. This helps to give practitioners the necessary ammunition to solve problems quickly, at the expense of requiring the reader to trust us with some curatorial decisions.

This book will teach deep learning concepts from scratch. Sometimes, we want to delve into fine details about the models that would typically be hidden from the user by deep learning frameworks' advanced abstractions. This comes up especially in the basic tutorials, where we want you to understand everything that happens in a given layer or optimizer. In these cases, we will often present two versions of the example: one where we implement everything from scratch, relying only on NumPy-like functionality and automatic differentiation, and another, more practical example, where we write succinct code using the high-level APIs of deep learning frameworks. Once we have taught you how some component works, we can just use the high-level APIs in subsequent tutorials.

Content and Structure

The book can be roughly divided into three parts, focusing on preliminaries, deep learning techniques, and advanced topics focused on real systems and applications (Fig. 1).

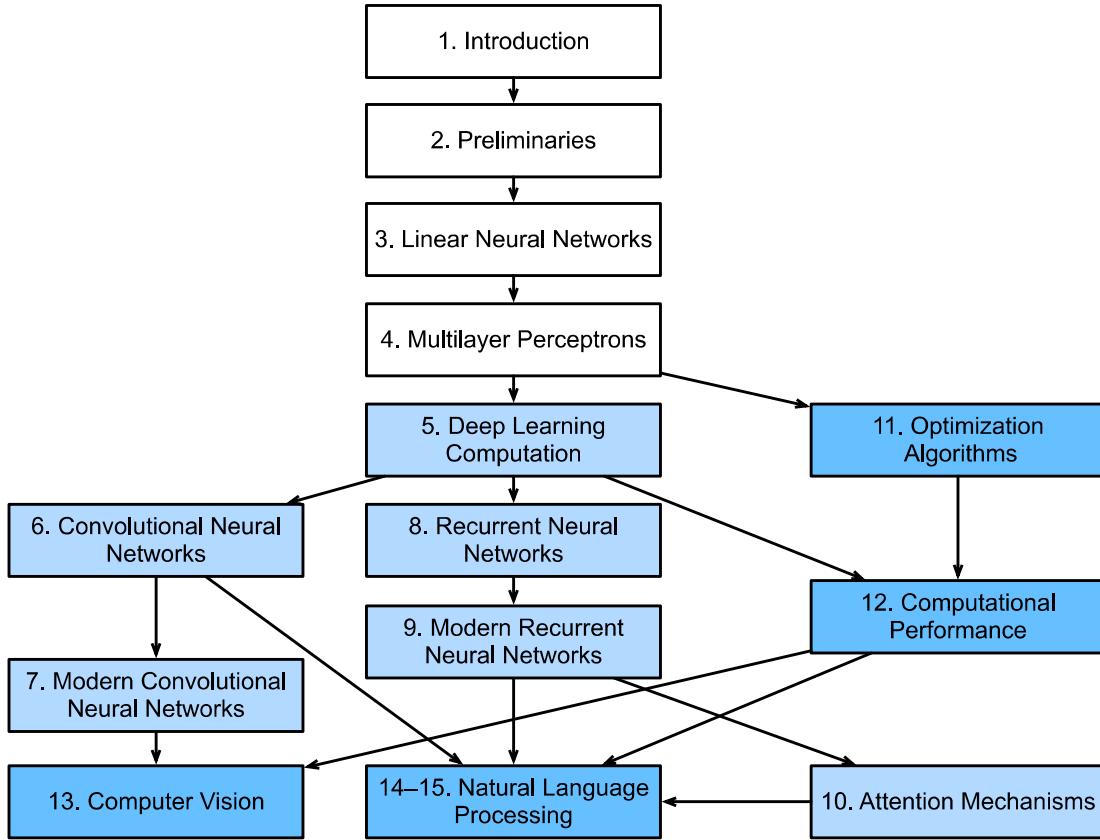


Fig. 1: Book structure

- The first part covers basics and preliminaries. [Chapter 1](#) offers an introduction to deep learning. Then, in [Chapter 2](#), we quickly bring you up to speed on the prerequisites required for hands-on deep learning, such as how to store and manipulate data, and how to apply various numerical operations based on basic concepts from linear algebra, calculus, and probability. [Chapter 3](#) and [Chapter 4](#) cover the most basic concepts and techniques in deep learning, including regression and classification; linear models and multilayer perceptrons; and overfitting and regularization.
- The next five chapters focus on modern deep learning techniques. [Chapter 5](#) describes the key computational components of deep learning systems and lays the groundwork for our subsequent implementations of more complex models. Next, [Chapter 6](#) and [Chapter 7](#), introduce convolutional neural networks (CNNs), powerful tools that form the backbone of most modern computer vision systems. Similarly, [Chapter 8](#) and [Chapter 9](#) introduce recurrent neural networks (RNNs), models that exploit sequential (e.g., temporal) structure in data and are commonly used for natural language processing and time series prediction. In [Chapter 10](#), we introduce a relatively new class of models based on so-called attention mechanisms that has displaced RNNs as the dominant architecture for most natural language processing tasks. These sections will bring you up to speed on the most powerful and general tools that are widely used by deep learning practitioners.
- Part three discusses scalability, efficiency, and applications. First, in [Chapter 11](#), we dis-

cuss several common optimization algorithms used to train deep learning models. The next chapter, [Chapter 12](#), examines several key factors that influence the computational performance of your deep learning code. In [Chapter 13](#), we illustrate major applications of deep learning in computer vision. In [Chapter 14](#) and [Chapter 15](#), we show how to pretrain language representation models and apply them to natural language processing tasks.

Code

Most sections of this book feature executable code. We believe that some intuitions are best developed via trial and error, tweaking the code in small ways and observing the results. Ideally, an elegant mathematical theory might tell us precisely how to tweak our code to achieve a desired result. However, today deep learning practitioners today must often tread where no cogent theory can provide firm guidance. Despite our best attempts, formal explanations for the efficacy of various techniques are still lacking, both because the mathematics to characterize these models can be so difficult and also because serious inquiry on these topics has only just recently kicked into high gear. We are hopeful that as the theory of deep learning progresses, future editions of this book can provide insights that eclipse those presently available.

To avoid unnecessary repetition, we encapsulate some of our most frequently imported and referred-to functions and classes in the d2l package. To indicate a block of code, such as a function, class, or collection of import statements, that will be subsequently accessed via the d2l package, we will mark it with `#@save`. We offer a detailed overview of these functions and classes in [Section 19.7](#). The d2l package is lightweight and only requires the following dependencies:

```
#@save
import collections
import hashlib
import math
import os
import random
import re
import shutil
import sys
import tarfile
import time
import zipfile
from collections import defaultdict
import pandas as pd
import requests
from IPython import display
from matplotlib import pyplot as plt

d2l = sys.modules[__name__]
```

Most of the code in this book is based on Apache MXNet, an open-source framework for deep learning that is the preferred choice of AWS (Amazon Web Services), as well as many colleges and companies. All of the code in this book has passed tests under the newest MXNet version. However, due to the rapid development of deep learning, some code *in the print edition* may not work properly in future versions of MXNet. We plan to keep the online version up-to-date. In case you encounter any problems, please consult [Installation](#) (page 9) to update your code and runtime environment.

Here is how we import modules from MXNet.

```
#@save
from mxnet import autograd, context, gluon, image, init, np, npx
from mxnet.gluon import nn, rnn
```

Target Audience

This book is for students (undergraduate or graduate), engineers, and researchers, who seek a solid grasp of the practical techniques of deep learning. Because we explain every concept from scratch, no previous background in deep learning or machine learning is required. Fully explaining the methods of deep learning requires some mathematics and programming, but we will only assume that you come in with some basics, including modest amounts of linear algebra, calculus, probability, and Python programming. Just in case you forgot the basics, the Appendix provides a refresher on most of the mathematics you will find in this book. Most of the time, we will prioritize intuition and ideas over mathematical rigor. If you would like to extend these foundations beyond the prerequisites to understand our book, we happily recommend some other terrific resources: Linear Analysis by Bela Bollobas ([Bollobas, 1999](#)) covers linear algebra and functional analysis in great depth. All of Statistics ([Wasserman, 2013](#)) provides a marvelous introduction to statistics. Joe Blitzsteins books and [courses](#)⁵ on probability and inference are pedagogical gems. And if you have not used Python before, you may want to peruse this [Python tutorial](#)⁶.

Forum

Associated with this book, we have launched a discussion forum, located at [discuss.d2l.ai](#)⁷. When you have questions on any section of the book, you can find a link to the associated discussion page at the end of each notebook.

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⁵ <https://projects.iq.harvard.edu/stat110/home>

⁶ <http://learnpython.org/>

⁷ <https://discuss.d2l.ai/>

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Summary

- Deep learning has revolutionized pattern recognition, introducing technology that now powers a wide range of technologies, including computer vision, natural language processing, automatic speech recognition.
- To successfully apply deep learning, you must understand how to cast a problem, the mathematics of modeling, the algorithms for fitting your models to data, and the engineering techniques to implement it all.
- This book presents a comprehensive resource, including prose, figures, mathematics, and code, all in one place.
- To answer questions related to this book, visit our forum at <https://discuss.d2l.ai/>.
- All notebooks are available for download on GitHub.

Exercises

1. Register an account on the discussion forum of this book discuss.d2l.ai⁸.
2. Install Python on your computer.
3. Follow the links at the bottom of the section to the forum, where you will be able to seek out help and discuss the book and find answers to your questions by engaging the authors and broader community.

⁸ <https://discuss.d2l.ai/>

Discussions⁹

⁹ <https://discuss.d2l.ai/t/18>

Installation

In order to get you up and running for hands-on learning experience, we need to set you up with an environment for running Python, Jupyter notebooks, the relevant libraries, and the code needed to run the book itself.

Installing Miniconda

The simplest way to get going will be to install [Miniconda¹⁰](#). The Python 3.x version is required. You can skip the following steps if conda has already been installed.

Visit the Miniconda website and determine the appropriate version for your system based on your Python 3.x version and machine architecture. For example, if you are using macOS and Python 3.x you would download the bash script with strings “Miniconda3” and “MacOSX” in its name, navigate to the download location and execute the installation as follows:

```
sh Miniconda3-latest-MacOSX-x86_64.sh -b
```

A Linux user with Python 3.x would download the file with strings “Miniconda3” and “Linux” in its name and execute the following at the download location:

```
sh Miniconda3-latest-Linux-x86_64.sh -b
```

Next, initialize the shell so we can run conda directly.

```
~/miniconda3/bin/conda init
```

Now close and re-open your current shell. You should be able to create a new environment as following:

```
conda create --name d2l python=3.8 -y
```

¹⁰ <https://conda.io/en/latest/miniconda.html>

Downloading the D2L Notebooks

Next, we need to download the code of this book. You can click the “All Notebooks” tab on the top of any HTML page to download and unzip the code. Alternatively, if you have `unzip` (otherwise run `sudo apt install unzip`) available:

```
mkdir d2l-en && cd d2l-en  
curl https://d2l.ai/d2l-en.zip -o d2l-en.zip  
unzip d2l-en.zip && rm d2l-en.zip
```

Now we will want to activate the `d2l` environment.

```
conda activate d2l
```

Installing the Framework and the `d2l` Package

Before installing the deep learning framework, please first check whether or not you have proper GPUs on your machine (the GPUs that power the display on a standard laptop do not count for our purposes). If you are installing on a GPU server, proceed to [GPU Support](#) (page 11) for instructions to install a GPU-supported version.

Otherwise, you can install the CPU version as follows. That will be more than enough horsepower to get you through the first few chapters but you will want to access GPUs before running larger models.

```
pip install mxnet==1.7.0.post1
```

We also install the `d2l` package that encapsulates frequently used functions and classes in this book.

```
# -U: Upgrade all packages to the newest available version  
pip install -U d2l
```

Once they are installed, we now open the Jupyter notebook by running:

```
jupyter notebook
```

At this point, you can open <http://localhost:8888> (it usually opens automatically) in your Web browser. Then we can run the code for each section of the book. Please always execute `conda activate d2l` to activate the runtime environment before running the code of the book or updating the deep learning framework or the `d2l` package. To exit the environment, run `conda deactivate`.

GPU Support

By default, MXNet is installed without GPU support to ensure that it will run on any computer (including most laptops). Part of this book requires or recommends running with GPU. If your computer has NVIDIA graphics cards and has installed CUDA¹¹, then you should install a GPU-enabled version. If you have installed the CPU-only version, you may need to remove it first by running:

```
pip uninstall mxnet
```

Then we need to find the CUDA version you installed. You may check it through nvcc --version or cat /usr/local/cuda/version.txt. Assume that you have installed CUDA 10.1, then you can install with the following command:

```
# For Windows users  
pip install mxnet-cu101==1.7.0 -f https://dist.mxnet.io/python  
  
# For Linux and macOS users  
pip install mxnet-cu101==1.7.0
```

You may change the last digits according to your CUDA version, e.g., cu100 for CUDA 10.0 and cu90 for CUDA 9.0.

Exercises

1. Download the code for the book and install the runtime environment.

Discussions¹²

¹¹ <https://developer.nvidia.com/cuda-downloads>

¹² <https://discuss.d2l.ai/t/23>

Notation

The notation used throughout this book is summarized below.

Numbers

- x : A scalar
- \mathbf{x} : A vector
- \mathbf{X} : A matrix
- X : A tensor
- \mathbf{I} : An identity matrix
- $x_i, [\mathbf{x}]_i$: The i^{th} element of vector \mathbf{x}
- $x_{ij}, x_{i,j}, [\mathbf{X}]_{ij}, [\mathbf{X}]_{i,j}$: The element of matrix \mathbf{X} at row i and column j

Set Theory

- \mathcal{X} : A set
- \mathbb{Z} : The set of integers
- \mathbb{Z}^+ : The set of positive integers
- \mathbb{R} : The set of real numbers
- \mathbb{R}^n : The set of n -dimensional vectors of real numbers
- $\mathbb{R}^{a \times b}$: The set of matrices of real numbers with a rows and b columns
- $|\mathcal{X}|$: Cardinality (number of elements) of set \mathcal{X}
- $\mathcal{A} \cup \mathcal{B}$: Union of sets \mathcal{A} and \mathcal{B}
- $\mathcal{A} \cap \mathcal{B}$: Intersection of sets \mathcal{A} and \mathcal{B}
- $\mathcal{A} \setminus \mathcal{B}$: Subtraction of set \mathcal{B} from set \mathcal{A}

Functions and Operators

- $f(\cdot)$: A function
- $\log(\cdot)$: The natural logarithm
- $\exp(\cdot)$: The exponential function
- $\mathbf{1}_{\mathcal{X}}$: The indicator function
- $(\cdot)^\top$: Transpose of a vector or a matrix
- \mathbf{X}^{-1} : Inverse of matrix \mathbf{X}
- \odot : Hadamard (elementwise) product
- $[\cdot, \cdot]$: Concatenation
- $|\mathcal{X}|$: Cardinality of set \mathcal{X}
- $\|\cdot\|_p$: L_p norm
- $\|\cdot\|$: L_2 norm
- $\langle \mathbf{x}, \mathbf{y} \rangle$: Dot product of vectors \mathbf{x} and \mathbf{y}
- \sum : Series addition
- \prod : Series multiplication
- $\stackrel{\text{def}}{=}$: Definition

Calculus

- $\frac{dy}{dx}$: Derivative of y with respect to x
- $\frac{\partial y}{\partial x}$: Partial derivative of y with respect to x
- $\nabla_{\mathbf{x}} y$: Gradient of y with respect to \mathbf{x}
- $\int_a^b f(x) dx$: Definite integral of f from a to b with respect to x
- $\int f(x) dx$: Indefinite integral of f with respect to x

Probability and Information Theory

- $P(\cdot)$: Probability distribution
- $z \sim P$: Random variable z has probability distribution P
- $P(X | Y)$: Conditional probability of $X | Y$
- $p(x)$: Probability density function
- $E_x[f(x)]$: Expectation of f with respect to x
- $X \perp Y$: Random variables X and Y are independent

- $X \perp Y \mid Z$: Random variables X and Y are conditionally independent given random variable Z
- $\text{Var}(X)$: Variance of random variable X
- σ_X : Standard deviation of random variable X
- $\text{Cov}(X, Y)$: Covariance of random variables X and Y
- $\rho(X, Y)$: Correlation of random variables X and Y
- $H(X)$: Entropy of random variable X
- $D_{\text{KL}}(P \parallel Q)$: KL-divergence of distributions P and Q

Complexity

- \mathcal{O} : Big O notation

Discussions¹³

¹³ <https://discuss.d2l.ai/t/25>

1 | Introduction

Until recently, nearly every computer program that we interact with daily was coded by software developers from first principles. Say that we wanted to write an application to manage an e-commerce platform. After huddling around a whiteboard for a few hours to ponder the problem, we would come up with the broad strokes of a working solution that might probably look something like this: (i) users interact with the application through an interface running in a web browser or mobile application; (ii) our application interacts with a commercial-grade database engine to keep track of each user's state and maintain records of historical transactions; and (iii) at the heart of our application, the *business logic* (you might say, the *brains*) of our application spells out in methodical detail the appropriate action that our program should take in every conceivable circumstance.

To build the brains of our application, we would have to step through every possible corner case that we anticipate encountering, devising appropriate rules. Each time a customer clicks to add an item to their shopping cart, we add an entry to the shopping cart database table, associating that user's ID with the requested product's ID. While few developers ever get it completely right the first time (it might take some test runs to work out the kinks), for the most part, we could write such a program from first principles and confidently launch it *before* ever seeing a real customer. Our ability to design automated systems from first principles that drive functioning products and systems, often in novel situations, is a remarkable cognitive feat. And when you are able to devise solutions that work 100% of the time, you should not be using machine learning.

Fortunately for the growing community of machine learning scientists, many tasks that we would like to automate do not bend so easily to human ingenuity. Imagine huddling around the whiteboard with the smartest minds you know, but this time you are tackling one of the following problems:

- Write a program that predicts tomorrow's weather given geographic information, satellite images, and a trailing window of past weather.
- Write a program that takes in a question, expressed in free-form text, and answers it correctly.
- Write a program that given an image can identify all the people it contains, drawing outlines around each.
- Write a program that presents users with products that they are likely to enjoy but unlikely, in the natural course of browsing, to encounter.

In each of these cases, even elite programmers are incapable of coding up solutions from scratch. The reasons for this can vary. Sometimes the program that we are looking for follows a pattern that changes over time, and we need our programs to adapt. In other cases, the relationship (say between pixels, and abstract categories) may be too complicated, requiring thousands or millions of computations that are beyond our conscious understanding even if our eyes manage the task

effortlessly. *Machine learning* is the study of powerful techniques that can learn from experience. As a machine learning algorithm accumulates more experience, typically in the form of observational data or interactions with an environment, its performance improves. Contrast this with our deterministic e-commerce platform, which performs according to the same business logic, no matter how much experience accrues, until the developers themselves learn and decide that it is time to update the software. In this book, we will teach you the fundamentals of machine learning, and focus in particular on *deep learning*, a powerful set of techniques driving innovations in areas as diverse as computer vision, natural language processing, healthcare, and genomics.

1.1 A Motivating Example

Before beginning writing, the authors of this book, like much of the work force, had to become caffeinated. We hopped in the car and started driving. Using an iPhone, Alex called out “Hey Siri”, awakening the phone’s voice recognition system. Then Mu commanded “directions to Blue Bottle coffee shop”. The phone quickly displayed the transcription of his command. It also recognized that we were asking for directions and launched the Maps application (app) to fulfill our request. Once launched, the Maps app identified a number of routes. Next to each route, the phone displayed a predicted transit time. While we fabricated this story for pedagogical convenience, it demonstrates that in the span of just a few seconds, our everyday interactions with a smart phone can engage several machine learning models.

Imagine just writing a program to respond to a *wake word* such as “Alexa”, “OK Google”, and “Hey Siri”. Try coding it up in a room by yourself with nothing but a computer and a code editor, as illustrated in Fig. 1.1.1. How would you write such a program from first principles? Think about it... the problem is hard. Every second, the microphone will collect roughly 44000 samples. Each sample is a measurement of the amplitude of the sound wave. What rule could map reliably from a snippet of raw audio to confident predictions {yes, no} on whether the snippet contains the wake word? If you are stuck, do not worry. We do not know how to write such a program from scratch either. That is why we use machine learning.

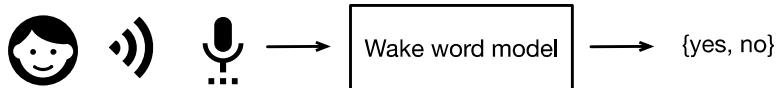


Fig. 1.1.1: Identify a wake word.

Here is the trick. Often, even when we do not know how to tell a computer explicitly how to map from inputs to outputs, we are nonetheless capable of performing the cognitive feat ourselves. In other words, even if you do not know how to program a computer to recognize the word “Alexa”, you yourself are able to recognize it. Armed with this ability, we can collect a huge *dataset* containing examples of audio and label those that do and that do not contain the wake word. In the machine learning approach, we do not attempt to design a system *explicitly* to recognize wake words. Instead, we define a flexible program whose behavior is determined by a number of *parameters*. Then we use the dataset to determine the best possible set of parameters, those that improve the performance of our program with respect to some measure of performance on the task of interest.

You can think of the parameters as knobs that we can turn, manipulating the behavior of the program. Fixing the parameters, we call the program a *model*. The set of all distinct programs

(input-output mappings) that we can produce just by manipulating the parameters is called a *family* of models. And the meta-program that uses our dataset to choose the parameters is called a *learning algorithm*.

Before we can go ahead and engage the learning algorithm, we have to define the problem precisely, pinning down the exact nature of the inputs and outputs, and choosing an appropriate model family. In this case, our model receives a snippet of audio as *input*, and the model generates a selection among {yes, no} as *output*. If all goes according to plan the model's guesses will typically be correct as to whether the snippet contains the wake word.

If we choose the right family of models, there should exist one setting of the knobs such that the model fires “yes” every time it hears the word “Alexa”. Because the exact choice of the wake word is arbitrary, we will probably need a model family sufficiently rich that, via another setting of the knobs, it could fire “yes” only upon hearing the word “Apricot”. We expect that the same model family should be suitable for “Alexa” recognition and “Apricot” recognition because they seem, intuitively, to be similar tasks. However, we might need a different family of models entirely if we want to deal with fundamentally different inputs or outputs, say if we wanted to map from images to captions, or from English sentences to Chinese sentences.

As you might guess, if we just set all of the knobs randomly, it is unlikely that our model will recognize “Alexa”, “Apricot”, or any other English word. In machine learning, the *learning* is the process by which we discover the right setting of the knobs coercing the desired behavior from our model. In other words, we *train* our model with data. As shown in Fig. 1.1.2, the training process usually looks like the following:

1. Start off with a randomly initialized model that cannot do anything useful.
2. Grab some of your data (e.g., audio snippets and corresponding {yes, no} labels).
3. Tweak the knobs so the model sucks less with respect to those examples.
4. Repeat Step 2 and 3 until the model is awesome.

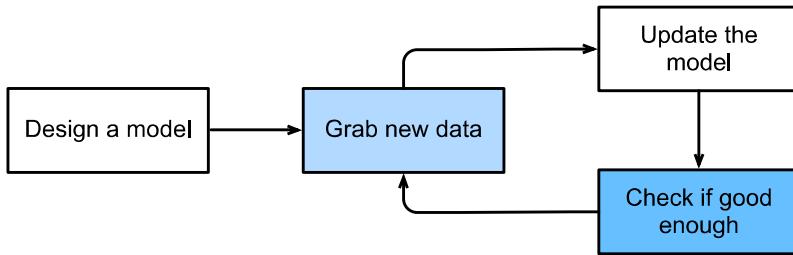


Fig. 1.1.2: A typical training process.

To summarize, rather than code up a wake word recognizer, we code up a program that can *learn* to recognize wake words, if we present it with a large labeled dataset. You can think of this act of determining a program’s behavior by presenting it with a dataset as *programming with data*. That is to say, we can “program” a cat detector by providing our machine learning system with many examples of cats and dogs. This way the detector will eventually learn to emit a very large positive number if it is a cat, a very large negative number if it is a dog, and something closer to zero if it is not sure, and this barely scratches the surface of what machine learning can do. Deep learning, which we will explain in greater detail later, is just one among many popular methods for solving machine learning problems.

1.2 Key Components

In our wake word example, we described a dataset consisting of audio snippets and binary labels, and we gave a hand-wavy sense of how we might train a model to approximate a mapping from snippets to classifications. This sort of problem, where we try to predict a designated unknown label based on known inputs given a dataset consisting of examples for which the labels are known, is called *supervised learning*. This is just one among many kinds of machine learning problems. Later we will take a deep dive into different machine learning problems. First, we would like to shed more light on some core components that will follow us around, no matter what kind of machine learning problem we take on:

1. The *data* that we can learn from.
2. A *model* of how to transform the data.
3. An *objective function* that quantifies how well (or badly) the model is doing.
4. An *algorithm* to adjust the model's parameters to optimize the objective function.

1.2.1 Data

It might go without saying that you cannot do data science without data. We could lose hundreds of pages pondering what precisely constitutes data, but for now, we will err on the practical side and focus on the key properties to be concerned with. Generally, we are concerned with a collection of examples. In order to work with data usefully, we typically need to come up with a suitable numerical representation. Each *example* (or *data point*, *data instance*, *sample*) typically consists of a set of attributes called *features* (or *covariates*), from which the model must make its predictions. In the supervised learning problems above, the thing to predict is a special attribute that is designated as the *label* (or *target*).

If we were working with image data, each individual photograph might constitute an example, each represented by an ordered list of numerical values corresponding to the brightness of each pixel. A 200×200 color photograph would consist of $200 \times 200 \times 3 = 120000$ numerical values, corresponding to the brightness of the red, green, and blue channels for each spatial location. In another traditional task, we might try to predict whether or not a patient will survive, given a standard set of features such as age, vital signs, and diagnoses.

When every example is characterized by the same number of numerical values, we say that the data consist of fixed-length vectors and we describe the constant length of the vectors as the *dimensionality* of the data. As you might imagine, fixed-length can be a convenient property. If we wanted to train a model to recognize cancer in microscopy images, fixed-length inputs mean we have one less thing to worry about.

However, not all data can easily be represented as *fixed-length* vectors. While we might expect microscope images to come from standard equipment, we cannot expect images mined from the Internet to all show up with the same resolution or shape. For images, we might consider cropping them all to a standard size, but that strategy only gets us so far. We risk losing information in the cropped out portions. Moreover, text data resist fixed-length representations even more stubbornly. Consider the customer reviews left on e-commerce sites such as Amazon, IMDB, and TripAdvisor. Some are short: “it stinks!”. Others ramble for pages. One major advantage of deep learning over traditional methods is the comparative grace with which modern models can handle *varying-length* data.

Generally, the more data we have, the easier our job becomes. When we have more data, we can train more powerful models and rely less heavily on pre-conceived assumptions. The regime change from (comparatively) small to big data is a major contributor to the success of modern deep learning. To drive the point home, many of the most exciting models in deep learning do not work without large datasets. Some others work in the small data regime, but are no better than traditional approaches.

Finally, it is not enough to have lots of data and to process it cleverly. We need the *right* data. If the data are full of mistakes, or if the chosen features are not predictive of the target quantity of interest, learning is going to fail. The situation is captured well by the cliché: *garbage in, garbage out*. Moreover, poor predictive performance is not the only potential consequence. In sensitive applications of machine learning, like predictive policing, resume screening, and risk models used for lending, we must be especially alert to the consequences of garbage data. One common failure mode occurs in datasets where some groups of people are unrepresented in the training data. Imagine applying a skin cancer recognition system in the wild that had never seen black skin before. Failure can also occur when the data do not merely under-represent some groups but reflect societal prejudices. For example, if past hiring decisions are used to train a predictive model that will be used to screen resumes, then machine learning models could inadvertently capture and automate historical injustices. Note that this can all happen without the data scientist actively conspiring, or even being aware.

1.2.2 Models

Most machine learning involves transforming the data in some sense. We might want to build a system that ingests photos and predicts smiley-ness. Alternatively, we might want to ingest a set of sensor readings and predict how normal vs. anomalous the readings are. By *model*, we denote the computational machinery for ingesting data of one type, and spitting out predictions of a possibly different type. In particular, we are interested in statistical models that can be estimated from data. While simple models are perfectly capable of addressing appropriately simple problems, the problems that we focus on in this book stretch the limits of classical methods. Deep learning is differentiated from classical approaches principally by the set of powerful models that it focuses on. These models consist of many successive transformations of the data that are chained together top to bottom, thus the name *deep learning*. On our way to discussing deep models, we will also discuss some more traditional methods.

1.2.3 Objective Functions

Earlier, we introduced machine learning as learning from experience. By *learning* here, we mean improving at some task over time. But who is to say what constitutes an improvement? You might imagine that we could propose to update our model, and some people might disagree on whether the proposed update constituted an improvement or a decline.

In order to develop a formal mathematical system of learning machines, we need to have formal measures of how good (or bad) our models are. In machine learning, and optimization more generally, we call these *objective functions*. By convention, we usually define objective functions so that lower is better. This is merely a convention. You can take any function for which higher is better, and turn it into a new function that is qualitatively identical but for which lower is better by flipping the sign. Because lower is better, these functions are sometimes called *loss functions*.

When trying to predict numerical values, the most common loss function is *squared error*, i.e., the square of the difference between the prediction and the ground-truth. For classification, the most

common objective is to minimize error rate, i.e., the fraction of examples on which our predictions disagree with the ground truth. Some objectives (e.g., squared error) are easy to optimize. Others (e.g., error rate) are difficult to optimize directly, owing to non-differentiability or other complications. In these cases, it is common to optimize a *surrogate objective*.

Typically, the loss function is defined with respect to the model's parameters and depends upon the dataset. We learn the best values of our model's parameters by minimizing the loss incurred on a set consisting of some number of examples collected for training. However, doing well on the training data does not guarantee that we will do well on unseen data. So we will typically want to split the available data into two partitions: the *training dataset* (or *training set*, for fitting model parameters) and the *test dataset* (or *test set*, which is held out for evaluation), reporting how the model performs on both of them. You could think of training performance as being like a student's scores on practice exams used to prepare for some real final exam. Even if the results are encouraging, that does not guarantee success on the final exam. In other words, the test performance can deviate significantly from the training performance. When a model performs well on the training set but fails to generalize to unseen data, we say that it is *overfitting*. In real-life terms, this is like flunking the real exam despite doing well on practice exams.

1.2.4 Optimization Algorithms

Once we have got some data source and representation, a model, and a well-defined objective function, we need an algorithm capable of searching for the best possible parameters for minimizing the loss function. Popular optimization algorithms for deep learning are based on an approach called *gradient descent*. In short, at each step, this method checks to see, for each parameter, which way the training set loss would move if you perturbed that parameter just a small amount. It then updates the parameter in the direction that may reduce the loss.

1.3 Kinds of Machine Learning Problems

The wake word problem in our motivating example is just one among many problems that machine learning can tackle. To motivate the reader further and provide us with some common language when we talk about more problems throughout the book, in the following we list a sampling of machine learning problems. We will constantly refer to our aforementioned concepts such as data, models, and training techniques.

1.3.1 Supervised Learning

Supervised learning addresses the task of predicting labels given input features. Each feature-label pair is called an example. Sometimes, when the context is clear, we may use the term *examples* to refer to a collection of inputs, even when the corresponding labels are unknown. Our goal is to produce a model that maps any input to a label prediction.

To ground this description in a concrete example, if we were working in healthcare, then we might want to predict whether or not a patient would have a heart attack. This observation, “heart attack” or “no heart attack”, would be our label. The input features might be vital signs such as heart rate, diastolic blood pressure, and systolic blood pressure.

The supervision comes into play because for choosing the parameters, we (the supervisors) provide the model with a dataset consisting of labeled examples, where each example is matched with

the ground-truth label. In probabilistic terms, we typically are interested in estimating the conditional probability of a label given input features. While it is just one among several paradigms within machine learning, supervised learning accounts for the majority of successful applications of machine learning in industry. Partly, that is because many important tasks can be described crisply as estimating the probability of something unknown given a particular set of available data:

- Predict cancer vs. not cancer, given a computer tomography image.
- Predict the correct translation in French, given a sentence in English.
- Predict the price of a stock next month based on this month's financial reporting data.

Even with the simple description “predicting labels given input features” supervised learning can take a great many forms and require a great many modeling decisions, depending on (among other considerations) the type, size, and the number of inputs and outputs. For example, we use different models to process sequences of arbitrary lengths and for processing fixed-length vector representations. We will visit many of these problems in depth throughout this book.

Informally, the learning process looks something like the following. First, grab a big collection of examples for which the features are known and select from them a random subset, acquiring the ground-truth labels for each. Sometimes these labels might be available data that have already been collected (e.g., did a patient die within the following year?) and other times we might need to employ human annotators to label the data, (e.g., assigning images to categories). Together, these inputs and corresponding labels comprise the training set. We feed the training dataset into a supervised learning algorithm, a function that takes as input a dataset and outputs another function: the learned model. Finally, we can feed previously unseen inputs to the learned model, using its outputs as predictions of the corresponding label. The full process is drawn in Fig. 1.3.1.

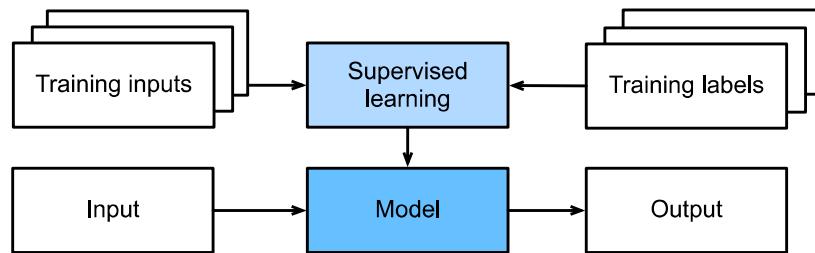


Fig. 1.3.1: Supervised learning.

Regression

Perhaps the simplest supervised learning task to wrap your head around is *regression*. Consider, for example, a set of data harvested from a database of home sales. We might construct a table, where each row corresponds to a different house, and each column corresponds to some relevant attribute, such as the square footage of a house, the number of bedrooms, the number of bathrooms, and the number of minutes (walking) to the center of town. In this dataset, each example would be a specific house, and the corresponding feature vector would be one row in the table. If you live in New York or San Francisco, and you are not the CEO of Amazon, Google, Microsoft, or Facebook, the (sq. footage, no. of bedrooms, no. of bathrooms, walking distance) feature vector for your home might look something like: [600, 1, 1, 60]. However, if you live in Pittsburgh, it might look more like [3000, 4, 3, 10]. Feature vectors like this are essential for most classic machine learning algorithms.

What makes a problem a regression is actually the output. Say that you are in the market for a

new home. You might want to estimate the fair market value of a house, given some features like above. The label, the price of sale, is a numerical value. When labels take on arbitrary numerical values, we call this a *regression* problem. Our goal is to produce a model whose predictions closely approximate the actual label values.

Lots of practical problems are well-described regression problems. Predicting the rating that a user will assign to a movie can be thought of as a regression problem and if you designed a great algorithm to accomplish this feat in 2009, you might have won the [1-million-dollar Netflix prize¹⁴](#). Predicting the length of stay for patients in the hospital is also a regression problem. A good rule of thumb is that any *how much?* or *how many?* problem should suggest regression, such as:

- How many hours will this surgery take?
- How much rainfall will this town have in the next six hours?

Even if you have never worked with machine learning before, you have probably worked through a regression problem informally. Imagine, for example, that you had your drains repaired and that your contractor spent 3 hours removing gunk from your sewage pipes. Then he sent you a bill of 350 dollars. Now imagine that your friend hired the same contractor for 2 hours and that he received a bill of 250 dollars. If someone then asked you how much to expect on their upcoming gunk-removal invoice you might make some reasonable assumptions, such as more hours worked costs more dollars. You might also assume that there is some base charge and that the contractor then charges per hour. If these assumptions held true, then given these two data examples, you could already identify the contractor's pricing structure: 100 dollars per hour plus 50 dollars to show up at your house. If you followed that much then you already understand the high-level idea behind linear regression.

In this case, we could produce the parameters that exactly matched the contractor's prices. Sometimes this is not possible, e.g., if some of the variance owes to a few factors besides your two features. In these cases, we will try to learn models that minimize the distance between our predictions and the observed values. In most of our chapters, we will focus on minimizing the squared error loss function. As we will see later, this loss corresponds to the assumption that our data were corrupted by Gaussian noise.

Classification

While regression models are great for addressing *how many?* questions, lots of problems do not bend comfortably to this template. For example, a bank wants to add check scanning to its mobile app. This would involve the customer snapping a photo of a check with their smart phone's camera and the app would need to be able to automatically understand text seen in the image. Specifically, it would also need to understand handwritten text to be even more robust, such as mapping a handwritten character to one of the known characters. This kind of *which one?* problem is called *classification*. It is treated with a different set of algorithms than those used for regression although many techniques will carry over.

In *classification*, we want our model to look at features, e.g., the pixel values in an image, and then predict which *category* (formally called *class*), among some discrete set of options, an example belongs. For handwritten digits, we might have ten classes, corresponding to the digits 0 through 9. The simplest form of classification is when there are only two classes, a problem which we call *binary classification*. For example, our dataset could consist of images of animals and our labels might be the classes {cat, dog}. While in regression, we sought a regressor to output a numerical value, in classification, we seek a classifier, whose output is the predicted class assignment.

¹⁴ https://en.wikipedia.org/wiki/Netflix_Prize

For reasons that we will get into as the book gets more technical, it can be hard to optimize a model that can only output a hard categorical assignment, e.g., either “cat” or “dog”. In these cases, it is usually much easier to instead express our model in the language of probabilities. Given features of an example, our model assigns a probability to each possible class. Returning to our animal classification example where the classes are {cat, dog}, a classifier might see an image and output the probability that the image is a cat as 0.9. We can interpret this number by saying that the classifier is 90% sure that the image depicts a cat. The magnitude of the probability for the predicted class conveys one notion of uncertainty. It is not the only notion of uncertainty and we will discuss others in more advanced chapters.

When we have more than two possible classes, we call the problem *multiclass classification*. Common examples include hand-written character recognition {0, 1, 2, ...9, a, b, c, ...}. While we attacked regression problems by trying to minimize the squared error loss function, the common loss function for classification problems is called *cross-entropy*, whose name can be demystified via an introduction to information theory in subsequent chapters.

Note that the most likely class is not necessarily the one that you are going to use for your decision. Assume that you find a beautiful mushroom in your backyard as shown in Fig. 1.3.2.



Fig. 1.3.2: Death cap—do not eat!

Now, assume that you built a classifier and trained it to predict if a mushroom is poisonous based on a photograph. Say our poison-detection classifier outputs that the probability that Fig. 1.3.2 contains a death cap is 0.2. In other words, the classifier is 80% sure that our mushroom is not a death cap. Still, you would have to be a fool to eat it. That is because the certain benefit of a delicious dinner is not worth a 20% risk of dying from it. In other words, the effect of the uncertain risk outweighs the benefit by far. Thus, we need to compute the expected risk that we incur as the loss function, i.e., we need to multiply the probability of the outcome with the benefit (or harm) associated with it. In this case, the loss incurred by eating the mushroom can be $0.2 \times \infty + 0.8 \times 0 = \infty$, whereas the loss of discarding it is $0.2 \times 0 + 0.8 \times 1 = 0.8$. Our caution was justified: as any mycologist would tell us, the mushroom in Fig. 1.3.2 actually is a death cap.

Classification can get much more complicated than just binary, multiclass, or even multi-label classification. For instance, there are some variants of classification for addressing hierarchies. Hierarchies assume that there exist some relationships among the many classes. So not all errors are equal—if we must err, we would prefer to misclassify to a related class rather than to a distant class. Usually, this is referred to as *hierarchical classification*. One early example is due to Linnaeus¹⁵, who organized the animals in a hierarchy.

¹⁵ https://en.wikipedia.org/wiki/Carl_Linnaeus

In the case of animal classification, it might not be so bad to mistake a poodle (a dog breed) for a schnauzer (another dog breed), but our model would pay a huge penalty if it confused a poodle for a dinosaur. Which hierarchy is relevant might depend on how you plan to use the model. For example, rattle snakes and garter snakes might be close on the phylogenetic tree, but mistaking a rattler for a garter could be deadly.

Tagging

Some classification problems fit neatly into the binary or multiclass classification setups. For example, we could train a normal binary classifier to distinguish cats from dogs. Given the current state of computer vision, we can do this easily, with off-the-shelf tools. Nonetheless, no matter how accurate our model gets, we might find ourselves in trouble when the classifier encounters an image of the *Town Musicians of Bremen*, a popular German fairy tale featuring four animals in Fig. 1.3.3.



Fig. 1.3.3: A donkey, a dog, a cat, and a rooster.

As you can see, there is a cat in Fig. 1.3.3, and a rooster, a dog, and a donkey, with some trees in the background. Depending on what we want to do with our model ultimately, treating this as a binary classification problem might not make a lot of sense. Instead, we might want to give the model the option of saying the image depicts a cat, a dog, a donkey, *and* a rooster.

The problem of learning to predict classes that are not mutually exclusive is called *multi-label classification*. Auto-tagging problems are typically best described as multi-label classification problems. Think of the tags people might apply to posts on a technical blog, e.g., “machine learning”, “technology”, “gadgets”, “programming languages”, “Linux”, “cloud computing”, “AWS”. A typical article might have 5–10 tags applied because these concepts are correlated. Posts about “cloud

computing” are likely to mention “AWS” and posts about “machine learning” could also deal with “programming languages”.

We also have to deal with this kind of problem when dealing with the biomedical literature, where correctly tagging articles is important because it allows researchers to do exhaustive reviews of the literature. At the National Library of Medicine, a number of professional annotators go over each article that gets indexed in PubMed to associate it with the relevant terms from MeSH, a collection of roughly 28000 tags. This is a time-consuming process and the annotators typically have a one-year lag between archiving and tagging. Machine learning can be used here to provide provisional tags until each article can have a proper manual review. Indeed, for several years, the BioASQ organization has [hosted competitions](#)¹⁶ to do precisely this.

Search

Sometimes we do not just want to assign each example to a bucket or to a real value. In the field of information retrieval, we want to impose a ranking on a set of items. Take web search for an example. The goal is less to determine whether a particular page is relevant for a query, but rather, which one of the plethora of search results is most relevant for a particular user. We really care about the ordering of the relevant search results and our learning algorithm needs to produce ordered subsets of elements from a larger set. In other words, if we are asked to produce the first 5 letters from the alphabet, there is a difference between returning “A B C D E” and “C A B E D”. Even if the result set is the same, the ordering within the set matters.

One possible solution to this problem is to first assign to every element in the set a corresponding relevance score and then to retrieve the top-rated elements. [PageRank](#)¹⁷, the original secret sauce behind the Google search engine was an early example of such a scoring system but it was peculiar in that it did not depend on the actual query. Here they relied on a simple relevance filter to identify the set of relevant items and then on PageRank to order those results that contained the query term. Nowadays, search engines use machine learning and behavioral models to obtain query-dependent relevance scores. There are entire academic conferences devoted to this subject.

Recommender Systems

Recommender systems are another problem setting that is related to search and ranking. The problems are similar insofar as the goal is to display a set of relevant items to the user. The main difference is the emphasis on *personalization* to specific users in the context of recommender systems. For instance, for movie recommendations, the results page for a science fiction fan and the results page for a connoisseur of Peter Sellers comedies might differ significantly. Similar problems pop up in other recommendation settings, e.g., for retail products, music, and news recommendation.

In some cases, customers provide explicit feedback communicating how much they liked a particular product (e.g., the product ratings and reviews on Amazon, IMDb, and GoodReads). In some other cases, they provide implicit feedback, e.g., by skipping titles on a playlist, which might indicate dissatisfaction but might just indicate that the song was inappropriate in context. In the simplest formulations, these systems are trained to estimate some score, such as an estimated rating or the probability of purchase, given a user and an item.

¹⁶ <http://bioasq.org/>

¹⁷ <https://en.wikipedia.org/wiki/PageRank>

Given such a model, for any given user, we could retrieve the set of objects with the largest scores, which could then be recommended to the user. Production systems are considerably more advanced and take detailed user activity and item characteristics into account when computing such scores. Fig. 1.3.4 is an example of deep learning books recommended by Amazon based on personalization algorithms tuned to capture one's preferences.

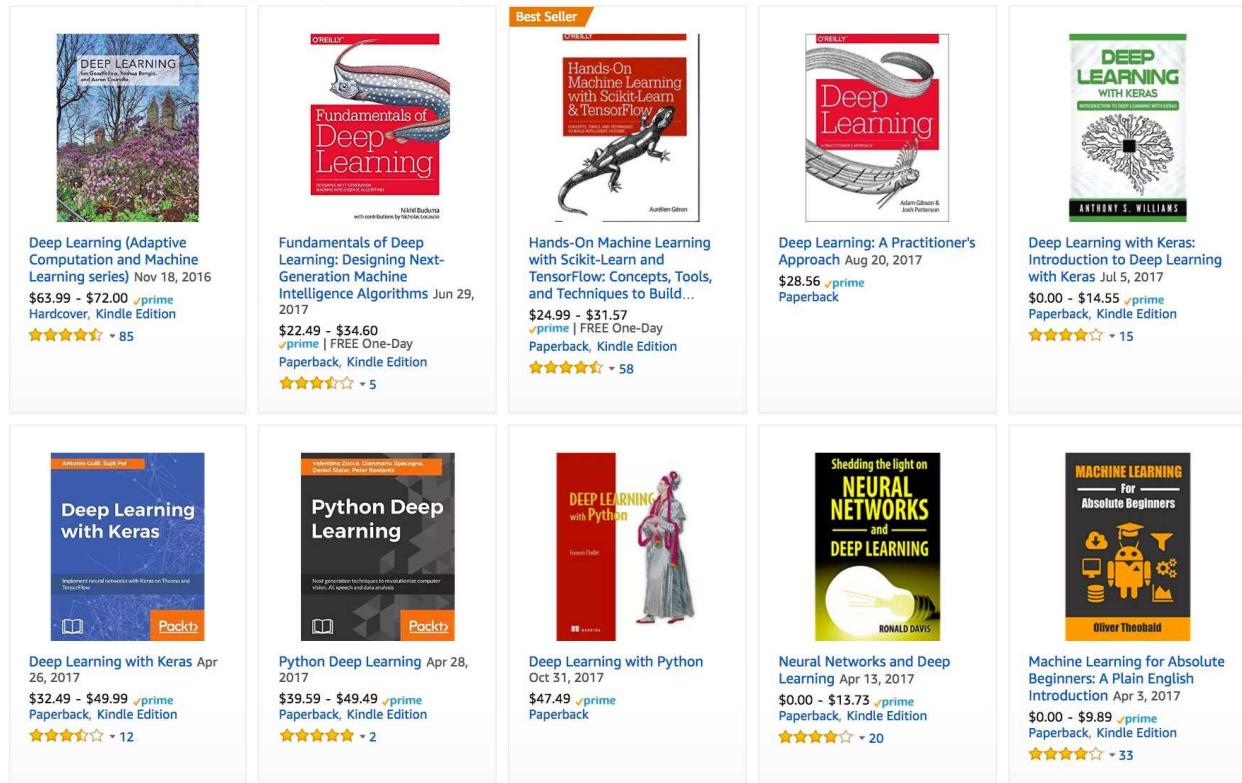


Fig. 1.3.4: Deep learning books recommended by Amazon.

Despite their tremendous economic value, recommendation systems naively built on top of predictive models suffer some serious conceptual flaws. To start, we only observe *censored feedback*: users preferentially rate movies that they feel strongly about. For example, on a five-point scale, you might notice that items receive many five and one star ratings but that there are conspicuously few three-star ratings. Moreover, current purchase habits are often a result of the recommendation algorithm currently in place, but learning algorithms do not always take this detail into account. Thus it is possible for feedback loops to form where a recommender system preferentially pushes an item that is then taken to be better (due to greater purchases) and in turn is recommended even more frequently. Many of these problems about how to deal with censoring, incentives, and feedback loops, are important open research questions.

Sequence Learning

So far, we have looked at problems where we have some fixed number of inputs and produce a fixed number of outputs. For example, we considered predicting house prices from a fixed set of features: square footage, number of bedrooms, number of bathrooms, walking time to downtown. We also discussed mapping from an image (of fixed dimension) to the predicted probabilities that it belongs to each of a fixed number of classes, or taking a user ID and a product ID, and predicting a star rating. In these cases, once we feed our fixed-length input into the model to generate an output, the model immediately forgets what it just saw.

This might be fine if our inputs truly all have the same dimensions and if successive inputs truly have nothing to do with each other. But how would we deal with video snippets? In this case, each snippet might consist of a different number of frames. And our guess of what is going on in each frame might be much stronger if we take into account the previous or succeeding frames. Same goes for language. One popular deep learning problem is machine translation: the task of ingesting sentences in some source language and predicting their translation in another language.

These problems also occur in medicine. We might want a model to monitor patients in the intensive care unit and to fire off alerts if their risk of death in the next 24 hours exceeds some threshold. We definitely would not want this model to throw away everything it knows about the patient history each hour and just make its predictions based on the most recent measurements.

These problems are among the most exciting applications of machine learning and they are instances of *sequence learning*. They require a model to either ingest sequences of inputs or to emit sequences of outputs (or both). Specifically, *sequence to sequence learning* considers problems where input and output are both variable-length sequences, such as machine translation and transcribing text from the spoken speech. While it is impossible to consider all types of sequence transformations, the following special cases are worth mentioning.

Tagging and Parsing. This involves annotating a text sequence with attributes. In other words, the number of inputs and outputs is essentially the same. For instance, we might want to know where the verbs and subjects are. Alternatively, we might want to know which words are the named entities. In general, the goal is to decompose and annotate text based on structural and grammatical assumptions to get some annotation. This sounds more complex than it actually is. Below is a very simple example of annotating a sentence with tags indicating which words refer to named entities (tagged as “Ent”).

```
Tom has dinner in Washington with Sally  
Ent - - - Ent - Ent
```

Automatic Speech Recognition. With speech recognition, the input sequence is an audio recording of a speaker (shown in Fig. 1.3.5), and the output is the textual transcript of what the speaker said. The challenge is that there are many more audio frames (sound is typically sampled at 8kHz or 16kHz) than text, i.e., there is no 1:1 correspondence between audio and text, since thousands of samples may correspond to a single spoken word. These are sequence to sequence learning problems where the output is much shorter than the input.

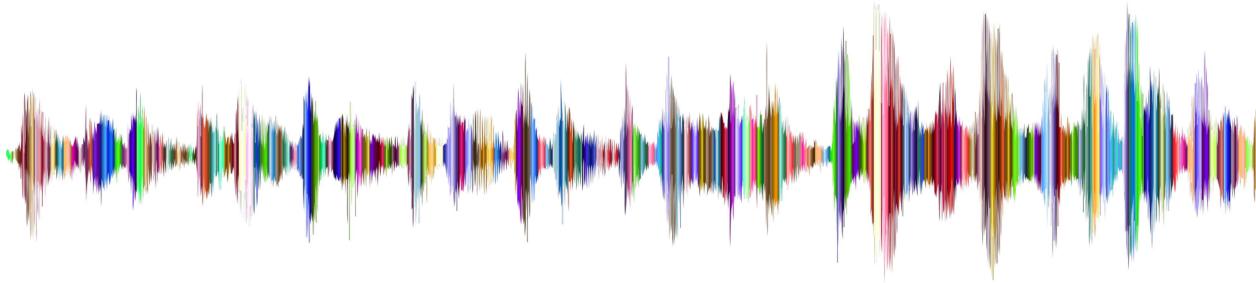


Fig. 1.3.5: -D-e-e-p- L-ea-r-ni-ng- in an audio recording.

Text to Speech. This is the inverse of automatic speech recognition. In other words, the input is text and the output is an audio file. In this case, the output is much longer than the input. While it is easy for humans to recognize a bad audio file, this is not quite so trivial for computers.

Machine Translation. Unlike the case of speech recognition, where corresponding inputs and outputs occur in the same order (after alignment), in machine translation, order inversion can be vital. In other words, while we are still converting one sequence into another, neither the number of inputs and outputs nor the order of corresponding data examples are assumed to be the same. Consider the following illustrative example of the peculiar tendency of Germans to place the verbs at the end of sentences.

German:	Haben Sie sich schon dieses grossartige Lehrwerk angeschaut?
English:	Did you already check out this excellent tutorial?
Wrong alignment:	Did you yourself already this excellent tutorial looked-at?

Many related problems pop up in other learning tasks. For instance, determining the order in which a user reads a webpage is a two-dimensional layout analysis problem. Dialogue problems exhibit all kinds of additional complications, where determining what to say next requires taking into account real-world knowledge and the prior state of the conversation across long temporal distances. These are active areas of research.

1.3.2 Unsupervised learning

All the examples so far were related to supervised learning, i.e., situations where we feed the model a giant dataset containing both the features and corresponding label values. You could think of the supervised learner as having an extremely specialized job and an extremely banal boss. The boss stands over your shoulder and tells you exactly what to do in every situation until you learn to map from situations to actions. Working for such a boss sounds pretty lame. On the other hand, it is easy to please this boss. You just recognize the pattern as quickly as possible and imitate their actions.

In a completely opposite way, it could be frustrating to work for a boss who has no idea what they want you to do. However, if you plan to be a data scientist, you had better get used to it. The boss might just hand you a giant dump of data and tell you to *do some data science with it!* This sounds vague because it is. We call this class of problems *unsupervised learning*, and the type and number of questions we could ask is limited only by our creativity. We will address unsupervised learning techniques in later chapters. To whet your appetite for now, we describe a few of the following questions you might ask.

- Can we find a small number of prototypes that accurately summarize the data? Given a set of photos, can we group them into landscape photos, pictures of dogs, babies, cats, and

mountain peaks? Likewise, given a collection of users' browsing activities, can we group them into users with similar behavior? This problem is typically known as *clustering*.

- Can we find a small number of parameters that accurately capture the relevant properties of the data? The trajectories of a ball are quite well described by velocity, diameter, and mass of the ball. Tailors have developed a small number of parameters that describe human body shape fairly accurately for the purpose of fitting clothes. These problems are referred to as *subspace estimation*. If the dependence is linear, it is called *principal component analysis*.
- Is there a representation of (arbitrarily structured) objects in Euclidean space such that symbolic properties can be well matched? This can be used to describe entities and their relations, such as "Rome" – "Italy" + "France" = "Paris".
- Is there a description of the root causes of much of the data that we observe? For instance, if we have demographic data about house prices, pollution, crime, location, education, and salaries, can we discover how they are related simply based on empirical data? The fields concerned with *causality* and *probabilistic graphical models* address this problem.
- Another important and exciting recent development in unsupervised learning is the advent of *generative adversarial networks*. These give us a procedural way to synthesize data, even complicated structured data like images and audio. The underlying statistical mechanisms are tests to check whether real and fake data are the same.

1.3.3 Interacting with an Environment

So far, we have not discussed where data actually come from, or what actually happens when a machine learning model generates an output. That is because supervised learning and unsupervised learning do not address these issues in a very sophisticated way. In either case, we grab a big pile of data upfront, then set our pattern recognition machines in motion without ever interacting with the environment again. Because all of the learning takes place after the algorithm is disconnected from the environment, this is sometimes called *offline learning*. For supervised learning, the process by considering data collection from an environment looks like Fig. 1.3.6.

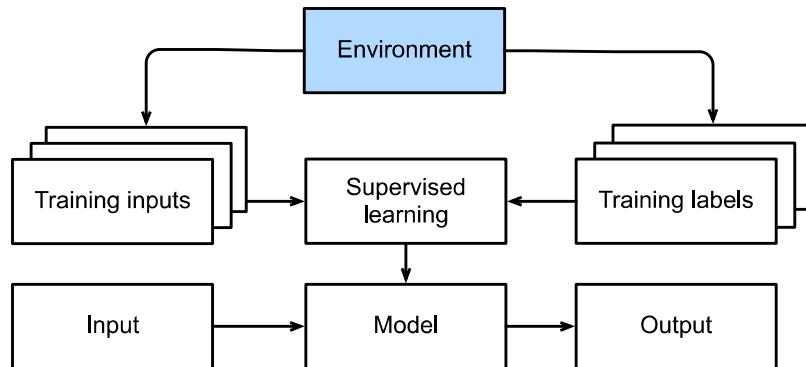


Fig. 1.3.6: Collecting data for supervised learning from an environment.

This simplicity of offline learning has its charms. The upside is that we can worry about pattern recognition in isolation, without any distraction from these other problems. But the downside is that the problem formulation is quite limiting. If you are more ambitious, or if you grew up reading Asimov's Robot series, then you might imagine artificially intelligent bots capable not only of making predictions, but also of taking actions in the world. We want to think about intelligent *agents*, not just predictive models. This means that we need to think about choosing *actions*, not

just making predictions. Moreover, unlike predictions, actions actually impact the environment. If we want to train an intelligent agent, we must account for the way its actions might impact the future observations of the agent.

Considering the interaction with an environment opens a whole set of new modeling questions. The following are just a few examples.

- Does the environment remember what we did previously?
- Does the environment want to help us, e.g., a user reading text into a speech recognizer?
- Does the environment want to beat us, i.e., an adversarial setting like spam filtering (against spammers) or playing a game (vs. an opponent)?
- Does the environment not care?
- Does the environment have shifting dynamics? For example, does future data always resemble the past or do the patterns change over time, either naturally or in response to our automated tools?

This last question raises the problem of *distribution shift*, when training and test data are different. It is a problem that most of us have experienced when taking exams written by a lecturer, while the homework was composed by his teaching assistants. Next, we will briefly describe reinforcement learning, a setting that explicitly considers interactions with an environment.

1.3.4 Reinforcement Learning

If you are interested in using machine learning to develop an agent that interacts with an environment and takes actions, then you are probably going to wind up focusing on *reinforcement learning*. This might include applications to robotics, to dialogue systems, and even to developing artificial intelligence (AI) for video games. *Deep reinforcement learning*, which applies deep learning to reinforcement learning problems, has surged in popularity. The breakthrough deep Q-network that beat humans at Atari games using only the visual input, and the AlphaGo program that dethroned the world champion at the board game Go are two prominent examples.

Reinforcement learning gives a very general statement of a problem, in which an agent interacts with an environment over a series of time steps. At each time step, the agent receives some *observation* from the environment and must choose an *action* that is subsequently transmitted back to the environment via some mechanism (sometimes called an actuator). Finally, the agent receives a reward from the environment. This process is illustrated in Fig. 1.3.7. The agent then receives a subsequent observation, and chooses a subsequent action, and so on. The behavior of an reinforcement learning agent is governed by a policy. In short, a *policy* is just a function that maps from observations of the environment to actions. The goal of reinforcement learning is to produce a good policy.

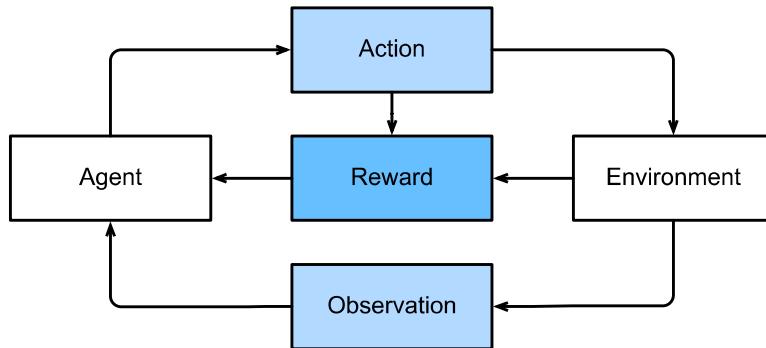


Fig. 1.3.7: The interaction between reinforcement learning and an environment.

It is hard to overstate the generality of the reinforcement learning framework. For example, we can cast any supervised learning problem as a reinforcement learning problem. Say we had a classification problem. We could create a reinforcement learning agent with one action corresponding to each class. We could then create an environment which gave a reward that was exactly equal to the loss function from the original supervised learning problem.

That being said, reinforcement learning can also address many problems that supervised learning cannot. For example, in supervised learning we always expect that the training input comes associated with the correct label. But in reinforcement learning, we do not assume that for each observation the environment tells us the optimal action. In general, we just get some reward. Moreover, the environment may not even tell us which actions led to the reward.

Consider for example the game of chess. The only real reward signal comes at the end of the game when we either win, which we might assign a reward of 1, or when we lose, which we could assign a reward of -1. So reinforcement learners must deal with the *credit assignment* problem: determining which actions to credit or blame for an outcome. The same goes for an employee who gets a promotion on October 11. That promotion likely reflects a large number of well-chosen actions over the previous year. Getting more promotions in the future requires figuring out what actions along the way led to the promotion.

Reinforcement learners may also have to deal with the problem of partial observability. That is, the current observation might not tell you everything about your current state. Say a cleaning robot found itself trapped in one of many identical closets in a house. Inferring the precise location (and thus state) of the robot might require considering its previous observations before entering the closet.

Finally, at any given point, reinforcement learners might know of one good policy, but there might be many other better policies that the agent has never tried. The reinforcement learner must constantly choose whether to *exploit* the best currently-known strategy as a policy, or to *explore* the space of strategies, potentially giving up some short-run reward in exchange for knowledge.

The general reinforcement learning problem is a very general setting. Actions affect subsequent observations. Rewards are only observed corresponding to the chosen actions. The environment may be either fully or partially observed. Accounting for all this complexity at once may ask too much of researchers. Moreover, not every practical problem exhibits all this complexity. As a result, researchers have studied a number of special cases of reinforcement learning problems.

When the environment is fully observed, we call the reinforcement learning problem a *Markov decision process*. When the state does not depend on the previous actions, we call the problem a *contextual bandit problem*. When there is no state, just a set of available actions with initially unknown rewards, this problem is the classic *multi-armed bandit problem*.

1.4 Roots

We have just reviewed a small subset of problems that machine learning can address. For a diverse set of machine learning problems, deep learning provides powerful tools for solving them. Although many deep learning methods are recent inventions, the core idea of programming with data and neural networks (names of many deep learning models) has been studied for centuries. In fact, humans have held the desire to analyze data and to predict future outcomes for long and much of natural science has its roots in this. For instance, the Bernoulli distribution is named after Jacob Bernoulli (1655–1705)¹⁸, and the Gaussian distribution was discovered by Carl Friedrich Gauss (1777–1855)¹⁹. He invented, for instance, the least mean squares algorithm, which is still used today for countless problems from insurance calculations to medical diagnostics. These tools gave rise to an experimental approach in the natural sciences—for instance, Ohm's law relating current and voltage in a resistor is perfectly described by a linear model.

Even in the middle ages, mathematicians had a keen intuition of estimates. For instance, the geometry book of Jacob Köbel (1460–1533)²⁰ illustrates averaging the length of 16 adult men's feet to obtain the average foot length.



Fig. 1.4.1: Estimating the length of a foot.

Fig. 1.4.1 illustrates how this estimator works. The 16 adult men were asked to line up in a row, when leaving the church. Their aggregate length was then divided by 16 to obtain an estimate for what now amounts to 1 foot. This “algorithm” was later improved to deal with misshapen feet—the 2 men with the shortest and longest feet respectively were sent away, averaging only over the remainder. This is one of the earliest examples of the trimmed mean estimate.

¹⁸ https://en.wikipedia.org/wiki/Jacob_Bernoulli

¹⁹ https://en.wikipedia.org/wiki/Carl_Friedrich_Gauss

²⁰ <https://www.maa.org/press/periodicals/convergence/mathematical-treasures-jacob-kobels-geometry>

Statistics really took off with the collection and availability of data. One of its titans, [Ronald Fisher \(1890–1962\)](#)²¹, contributed significantly to its theory and also its applications in genetics. Many of his algorithms (such as linear discriminant analysis) and formula (such as the Fisher information matrix) are still in frequent use today. In fact, even the Iris dataset that Fisher released in 1936 is still used sometimes to illustrate machine learning algorithms. He was also a proponent of eugenics, which should remind us that the morally dubious use of data science has as long and enduring a history as its productive use in industry and the natural sciences.

A second influence for machine learning came from information theory by [Claude Shannon \(1916–2001\)](#)²² and the theory of computation via [Alan Turing \(1912–1954\)](#)²³. Turing posed the question “can machines think?” in his famous paper *Computing Machinery and Intelligence* (Turing, 1950). In what he described as the Turing test, a machine can be considered *intelligent* if it is difficult for a human evaluator to distinguish between the replies from a machine and a human based on textual interactions.

Another influence can be found in neuroscience and psychology. After all, humans clearly exhibit intelligent behavior. It is thus only reasonable to ask whether one could explain and possibly reverse engineer this capacity. One of the oldest algorithms inspired in this fashion was formulated by [Donald Hebb \(1904–1985\)](#)²⁴. In his groundbreaking book *The Organization of Behavior* (Hebb & Hebb, 1949), he posited that neurons learn by positive reinforcement. This became known as the Hebbian learning rule. It is the prototype of Rosenblatt’s perceptron learning algorithm and it laid the foundations of many stochastic gradient descent algorithms that underpin deep learning today: reinforce desirable behavior and diminish undesirable behavior to obtain good settings of the parameters in a neural network.

Biological inspiration is what gave *neural networks* their name. For over a century (dating back to the models of Alexander Bain, 1873 and James Sherrington, 1890), researchers have tried to assemble computational circuits that resemble networks of interacting neurons. Over time, the interpretation of biology has become less literal but the name stuck. At its heart, lie a few key principles that can be found in most networks today:

- The alternation of linear and nonlinear processing units, often referred to as *layers*.
- The use of the chain rule (also known as *backpropagation*) for adjusting parameters in the entire network at once.

After initial rapid progress, research in neural networks languished from around 1995 until 2005. This was mainly due to two reasons. First, training a network is computationally very expensive. While random-access memory was plentiful at the end of the past century, computational power was scarce. Second, datasets were relatively small. In fact, Fisher’s Iris dataset from 1932 was a popular tool for testing the efficacy of algorithms. The MNIST dataset with its 60000 handwritten digits was considered huge.

Given the scarcity of data and computation, strong statistical tools such as kernel methods, decision trees and graphical models proved empirically superior. Unlike neural networks, they did not require weeks to train and provided predictable results with strong theoretical guarantees.

²¹ https://en.wikipedia.org/wiki/Ronald_Fisher

²² https://en.wikipedia.org/wiki/Claude_Shannon

²³ https://en.wikipedia.org/wiki/Alan_Turing

²⁴ https://en.wikipedia.org/wiki/Donald_O._Hebb

1.5 The Road to Deep Learning

Much of this changed with the ready availability of large amounts of data, due to the World Wide Web, the advent of companies serving hundreds of millions of users online, a dissemination of cheap, high-quality sensors, cheap data storage (Kryder’s law), and cheap computation (Moore’s law), in particular in the form of GPUs, originally engineered for computer gaming. Suddenly algorithms and models that seemed computationally infeasible became relevant (and vice versa). This is best illustrated in [Table 1.5.1](#).

Table 1.5.1: Dataset vs. computer memory and computational power

Decade	Dataset	Memory	Floating point calculations per second
1970	100 (Iris)	1 KB	100 KF (Intel 8080)
1980	1 K (House prices in Boston)	100 KB	1 MF (Intel 80186)
1990	10 K (optical character recognition)	10 MB	10 MF (Intel 80486)
2000	10 M (web pages)	100 MB	1 GF (Intel Core)
2010	10 G (advertising)	1 GB	1 TF (Nvidia C2050)
2020	1 T (social network)	100 GB	1 PF (Nvidia DGX-2)

It is evident that random-access memory has not kept pace with the growth in data. At the same time, the increase in computational power has outpaced that of the data available. This means that statistical models need to become more memory efficient (this is typically achieved by adding non-linearities) while simultaneously being able to spend more time on optimizing these parameters, due to an increased computational budget. Consequently, the sweet spot in machine learning and statistics moved from (generalized) linear models and kernel methods to deep neural networks. This is also one of the reasons why many of the mainstays of deep learning, such as multilayer perceptrons ([McCulloch & Pitts, 1943](#)), convolutional neural networks ([LeCun et al., 1998](#)), long short-term memory ([Hochreiter & Schmidhuber, 1997](#)), and Q-Learning ([Watkins & Dayan, 1992](#)), were essentially “rediscovered” in the past decade, after laying comparatively dormant for considerable time.

The recent progress in statistical models, applications, and algorithms has sometimes been likened to the Cambrian explosion: a moment of rapid progress in the evolution of species. Indeed, the state of the art is not just a mere consequence of available resources, applied to decades old algorithms. Note that the list below barely scratches the surface of the ideas that have helped researchers achieve tremendous progress over the past decade.

- Novel methods for capacity control, such as *dropout* ([Srivastava et al., 2014](#)), have helped to mitigate the danger of overfitting. This was achieved by applying noise injection ([Bishop, 1995](#)) throughout the neural network, replacing weights by random variables for training purposes.
- Attention mechanisms solved a second problem that had plagued statistics for over a century: how to increase the memory and complexity of a system without increasing the number of learnable parameters. Researchers found an elegant solution by using what can only be viewed as a learnable pointer structure ([Bahdanau et al., 2014](#)). Rather than having to remember an entire text sequence, e.g., for machine translation in a fixed-dimensional representation, all that needed to be stored was a pointer to the intermediate state of the translation process. This allowed for significantly increased accuracy for long sequences, since the model no longer needed to remember the entire sequence before commencing the generation of a new sequence.

- Multi-stage designs, e.g., via the memory networks (Sukhbaatar et al., 2015) and the neural programmer-interpreter (Reed & DeFreitas, 2015) allowed statistical modelers to describe iterative approaches to reasoning. These tools allow for an internal state of the deep neural network to be modified repeatedly, thus carrying out subsequent steps in a chain of reasoning, similar to how a processor can modify memory for a computation.
- Another key development was the invention of generative adversarial networks (Goodfellow et al., 2014). Traditionally, statistical methods for density estimation and generative models focused on finding proper probability distributions and (often approximate) algorithms for sampling from them. As a result, these algorithms were largely limited by the lack of flexibility inherent in the statistical models. The crucial innovation in generative adversarial networks was to replace the sampler by an arbitrary algorithm with differentiable parameters. These are then adjusted in such a way that the discriminator (effectively a two-sample test) cannot distinguish fake from real data. Through the ability to use arbitrary algorithms to generate data, it opened up density estimation to a wide variety of techniques. Examples of galloping Zebras (Zhu et al., 2017) and of fake celebrity faces (Karras et al., 2017) are both testimony to this progress. Even amateur doodlers can produce photorealistic images based on just sketches that describe how the layout of a scene looks like (Park et al., 2019).
- In many cases, a single GPU is insufficient to process the large amounts of data available for training. Over the past decade the ability to build parallel and distributed training algorithms has improved significantly. One of the key challenges in designing scalable algorithms is that the workhorse of deep learning optimization, stochastic gradient descent, relies on relatively small minibatches of data to be processed. At the same time, small batches limit the efficiency of GPUs. Hence, training on 1024 GPUs with a minibatch size of, say 32 images per batch amounts to an aggregate minibatch of about 32000 images. Recent work, first by Li (Li, 2017), and subsequently by (You et al., 2017) and (Jia et al., 2018) pushed the size up to 64000 observations, reducing training time for the ResNet-50 model on the ImageNet dataset to less than 7 minutes. For comparison—initially training times were measured in the order of days.
- The ability to parallelize computation has also contributed quite crucially to progress in reinforcement learning, at least whenever simulation is an option. This has led to significant progress in computers achieving superhuman performance in Go, Atari games, Starcraft, and in physics simulations (e.g., using MuJoCo). See e.g., (Silver et al., 2016) for a description of how to achieve this in AlphaGo. In a nutshell, reinforcement learning works best if plenty of (state, action, reward) triples are available, i.e., whenever it is possible to try out lots of things to learn how they relate to each other. Simulation provides such an avenue.
- Deep learning frameworks have played a crucial role in disseminating ideas. The first generation of frameworks allowing for easy modeling encompassed Caffe²⁵, Torch²⁶, and Theano²⁷. Many seminal papers were written using these tools. By now, they have been superseded by TensorFlow²⁸ (often used via its high level API Keras²⁹), CNTK³⁰, Caffe 2³¹, and Apache MXNet³². The third generation of tools, namely imperative tools for deep learning, was arguably spearheaded by Chainer³³, which used a syntax similar to Python NumPy to

²⁵ <https://github.com/BVLC/caffe>

²⁶ <https://github.com/torch>

²⁷ <https://github.com/Theano/Theano>

²⁸ <https://github.com/tensorflow/tensorflow>

²⁹ <https://github.com/keras-team/keras>

³⁰ <https://github.com/Microsoft/CNTK>

³¹ <https://github.com/caffe2/caffe2>

³² <https://github.com/apache/incubator-mxnet>

³³ <https://github.com/chainer/chainer>

describe models. This idea was adopted by both PyTorch³⁴, the Gluon API³⁵ of MXNet, and Jax³⁶.

The division of labor between system researchers building better tools and statistical modelers building better neural networks has greatly simplified things. For instance, training a linear logistic regression model used to be a nontrivial homework problem, worthy to give to new machine learning Ph.D. students at Carnegie Mellon University in 2014. By now, this task can be accomplished with less than 10 lines of code, putting it firmly into the grasp of programmers.

1.6 Success Stories

AI has a long history of delivering results that would be difficult to accomplish otherwise. For instance, the mail sorting systems using optical character recognition have been deployed since the 1990s. This is, after all, the source of the famous MNIST dataset of handwritten digits. The same applies to reading checks for bank deposits and scoring creditworthiness of applicants. Financial transactions are checked for fraud automatically. This forms the backbone of many e-commerce payment systems, such as PayPal, Stripe, AliPay, WeChat, Apple, Visa, and MasterCard. Computer programs for chess have been competitive for decades. Machine learning feeds search, recommendation, personalization, and ranking on the Internet. In other words, machine learning is pervasive, albeit often hidden from sight.

It is only recently that AI has been in the limelight, mostly due to solutions to problems that were considered intractable previously and that are directly related to consumers. Many of such advances are attributed to deep learning.

- Intelligent assistants, such as Apple’s Siri, Amazon’s Alexa, and Google’s assistant, are able to answer spoken questions with a reasonable degree of accuracy. This includes menial tasks such as turning on light switches (a boon to the disabled) up to making barber’s appointments and offering phone support dialog. This is likely the most noticeable sign that AI is affecting our lives.
- A key ingredient in digital assistants is the ability to recognize speech accurately. Gradually the accuracy of such systems has increased to the point where they reach human parity for certain applications (Xiong et al., 2018).
- Object recognition likewise has come a long way. Estimating the object in a picture was a fairly challenging task in 2010. On the ImageNet benchmark researchers from NEC Labs and University of Illinois at Urbana-Champaign achieved a top-5 error rate of 28% (Lin et al., 2010). By 2017, this error rate was reduced to 2.25% (Hu et al., 2018). Similarly, stunning results have been achieved for identifying birds or diagnosing skin cancer.
- Games used to be a bastion of human intelligence. Starting from TD-Gammon, a program for playing backgammon using temporal difference reinforcement learning, algorithmic and computational progress has led to algorithms for a wide range of applications. Unlike backgammon, chess has a much more complex state space and set of actions. DeepBlue beat Garry Kasparov using massive parallelism, special-purpose hardware and efficient search through the game tree (Campbell et al., 2002). Go is more difficult still, due to its huge state space. AlphaGo reached human parity in 2015, using deep learning combined with Monte Carlo tree sampling (Silver et al., 2016). The challenge in Poker was that the state space is

³⁴ <https://github.com/pytorch/pytorch>

³⁵ <https://github.com/apache/incubator-mxnet>

³⁶ <https://github.com/google/jax>

large and it is not fully observed (we do not know the opponents' cards). Libratus exceeded human performance in Poker using efficiently structured strategies (Brown & Sandholm, 2017). This illustrates the impressive progress in games and the fact that advanced algorithms played a crucial part in them.

- Another indication of progress in AI is the advent of self-driving cars and trucks. While full autonomy is not quite within reach yet, excellent progress has been made in this direction, with companies such as Tesla, NVIDIA, and Waymo shipping products that enable at least partial autonomy. What makes full autonomy so challenging is that proper driving requires the ability to perceive, to reason and to incorporate rules into a system. At present, deep learning is used primarily in the computer vision aspect of these problems. The rest is heavily tuned by engineers.

Again, the above list barely scratches the surface of where machine learning has impacted practical applications. For instance, robotics, logistics, computational biology, particle physics, and astronomy owe some of their most impressive recent advances at least in parts to machine learning. Machine learning is thus becoming a ubiquitous tool for engineers and scientists.

Frequently, the question of the AI apocalypse, or the AI singularity has been raised in non-technical articles on AI. The fear is that somehow machine learning systems will become sentient and decide independently from their programmers (and masters) about things that directly affect the livelihood of humans. To some extent, AI already affects the livelihood of humans in an immediate way: creditworthiness is assessed automatically, autopilots mostly navigate vehicles, decisions about whether to grant bail use statistical data as input. More frivolously, we can ask Alexa to switch on the coffee machine.

Fortunately, we are far from a sentient AI system that is ready to manipulate its human creators (or burn their coffee). First, AI systems are engineered, trained and deployed in a specific, goal-oriented manner. While their behavior might give the illusion of general intelligence, it is a combination of rules, heuristics and statistical models that underlie the design. Second, at present tools for *artificial general intelligence* simply do not exist that are able to improve themselves, reason about themselves, and that are able to modify, extend, and improve their own architecture while trying to solve general tasks.

A much more pressing concern is how AI is being used in our daily lives. It is likely that many menial tasks fulfilled by truck drivers and shop assistants can and will be automated. Farm robots will likely reduce the cost for organic farming but they will also automate harvesting operations. This phase of the industrial revolution may have profound consequences on large swaths of society, since truck drivers and shop assistants are some of the most common jobs in many countries. Furthermore, statistical models, when applied without care can lead to racial, gender, or age bias and raise reasonable concerns about procedural fairness if automated to drive consequential decisions. It is important to ensure that these algorithms are used with care. With what we know today, this strikes us a much more pressing concern than the potential of malevolent superintelligence to destroy humanity.

1.7 Characteristics

Thus far, we have talked about machine learning broadly, which is both a branch of AI and an approach to AI. Though deep learning is a subset of machine learning, the dizzying set of algorithms and applications makes it difficult to assess what specifically the ingredients for deep learning might be. This is as difficult as trying to pin down required ingredients for pizza since almost every component is substitutable.

As we have described, machine learning can use data to learn transformations between inputs and outputs, such as transforming audio into text in speech recognition. In doing so, it is often necessary to represent data in a way suitable for algorithms to transform such representations into the output. *Deep learning* is *deep* in precisely the sense that its models learn many *layers* of transformations, where each layer offers the representation at one level. For example, layers near the input may represent low-level details of the data, while layers closer to the classification output may represent more abstract concepts used for discrimination. Since *representation learning* aims at finding the representation itself, deep learning can be referred to as multi-level representation learning.

The problems that we have discussed so far, such as learning from the raw audio signal, the raw pixel values of images, or mapping between sentences of arbitrary lengths and their counterparts in foreign languages, are those where deep learning excels and where traditional machine learning methods falter. It turns out that these many-layered models are capable of addressing low-level perceptual data in a way that previous tools could not. Arguably the most significant commonality in deep learning methods is the use of *end-to-end training*. That is, rather than assembling a system based on components that are individually tuned, one builds the system and then tunes their performance jointly. For instance, in computer vision scientists used to separate the process of *feature engineering* from the process of building machine learning models. The Canny edge detector ([Canny, 1987](#)) and Lowe's SIFT feature extractor ([Lowe, 2004](#)) reigned supreme for over a decade as algorithms for mapping images into feature vectors. In bygone days, the crucial part of applying machine learning to these problems consisted of coming up with manually-engineered ways of transforming the data into some form amenable to shallow models. Unfortunately, there is only so little that humans can accomplish by ingenuity in comparison with a consistent evaluation over millions of choices carried out automatically by an algorithm. When deep learning took over, these feature extractors were replaced by automatically tuned filters, yielding superior accuracy.

Thus, one key advantage of deep learning is that it replaces not only the shallow models at the end of traditional learning pipelines, but also the labor-intensive process of feature engineering. Moreover, by replacing much of the domain-specific preprocessing, deep learning has eliminated many of the boundaries that previously separated computer vision, speech recognition, natural language processing, medical informatics, and other application areas, offering a unified set of tools for tackling diverse problems.

Beyond end-to-end training, we are experiencing a transition from parametric statistical descriptions to fully nonparametric models. When data are scarce, one needs to rely on simplifying assumptions about reality in order to obtain useful models. When data are abundant, this can be replaced by nonparametric models that fit reality more accurately. To some extent, this mirrors the progress that physics experienced in the middle of the previous century with the availability of computers. Rather than solving parametric approximations of how electrons behave by hand, one can now resort to numerical simulations of the associated partial differential equations. This has led to much more accurate models, albeit often at the expense of explainability.

Another difference to previous work is the acceptance of suboptimal solutions, dealing with non-

convex nonlinear optimization problems, and the willingness to try things before proving them. This newfound empiricism in dealing with statistical problems, combined with a rapid influx of talent has led to rapid progress of practical algorithms, albeit in many cases at the expense of modifying and re-inventing tools that existed for decades.

In the end, the deep learning community prides itself on sharing tools across academic and corporate boundaries, releasing many excellent libraries, statistical models, and trained networks as open source. It is in this spirit that the notebooks forming this book are freely available for distribution and use. We have worked hard to lower the barriers of access for everyone to learn about deep learning and we hope that our readers will benefit from this.

Summary

- Machine learning studies how computer systems can leverage experience (often data) to improve performance at specific tasks. It combines ideas from statistics, data mining, and optimization. Often, it is used as a means of implementing AI solutions.
- As a class of machine learning, representational learning focuses on how to automatically find the appropriate way to represent data. Deep learning is multi-level representation learning through learning many layers of transformations.
- Deep learning replaces not only the shallow models at the end of traditional machine learning pipelines, but also the labor-intensive process of feature engineering.
- Much of the recent progress in deep learning has been triggered by an abundance of data arising from cheap sensors and Internet-scale applications, and by significant progress in computation, mostly through GPUs.
- Whole system optimization is a key component in obtaining high performance. The availability of efficient deep learning frameworks has made design and implementation of this significantly easier.

Exercises

1. Which parts of code that you are currently writing could be “learned”, i.e., improved by learning and automatically determining design choices that are made in your code? Does your code include heuristic design choices?
2. Which problems that you encounter have many examples for how to solve them, yet no specific way to automate them? These may be prime candidates for using deep learning.
3. Viewing the development of AI as a new industrial revolution, what is the relationship between algorithms and data? Is it similar to steam engines and coal? What is the fundamental difference?
4. Where else can you apply the end-to-end training approach, such as in Fig. 1.1.2, physics, engineering, and econometrics?

Discussions³⁷

³⁷ <https://discuss.d2l.ai/t/22>

2 | Preliminaries

To get started with deep learning, we will need to develop a few basic skills. All machine learning is concerned with extracting information from data. So we will begin by learning the practical skills for storing, manipulating, and preprocessing data.

Moreover, machine learning typically requires working with large datasets, which we can think of as tables, where the rows correspond to examples and the columns correspond to attributes. Linear algebra gives us a powerful set of techniques for working with tabular data. We will not go too far into the weeds but rather focus on the basic of matrix operations and their implementation.

Additionally, deep learning is all about optimization. We have a model with some parameters and we want to find those that fit our data *the best*. Determining which way to move each parameter at each step of an algorithm requires a little bit of calculus, which will be briefly introduced. Fortunately, the autograd package automatically computes differentiation for us, and we will cover it next.

Next, machine learning is concerned with making predictions: what is the likely value of some unknown attribute, given the information that we observe? To reason rigorously under uncertainty we will need to invoke the language of probability.

In the end, the official documentation provides plenty of descriptions and examples that are beyond this book. To conclude the chapter, we will show you how to look up documentation for the needed information.

This book has kept the mathematical content to the minimum necessary to get a proper understanding of deep learning. However, it does not mean that this book is mathematics free. Thus, this chapter provides a rapid introduction to basic and frequently-used mathematics to allow anyone to understand at least *most* of the mathematical content of the book. If you wish to understand *all* of the mathematical content, further reviewing the [online appendix on mathematics³⁸](#) should be sufficient.

2.1 Data Manipulation

In order to get anything done, we need some way to store and manipulate data. Generally, there are two important things we need to do with data: (i) acquire them; and (ii) process them once they are inside the computer. There is no point in acquiring data without some way to store it, so let us get our hands dirty first by playing with synthetic data. To start, we introduce the n -dimensional array, which is also called the *tensor*.

If you have worked with NumPy, the most widely-used scientific computing package in Python, then you will find this section familiar. No matter which framework you use, its *tensor class*

³⁸ https://d2l.ai/chapter_appendix-mathematics-for-deep-learning/index.html

(ndarray in MXNet, Tensor in both PyTorch and TensorFlow) is similar to NumPy's ndarray with a few killer features. First, GPU is well-supported to accelerate the computation whereas NumPy only supports CPU computation. Second, the tensor class supports automatic differentiation. These properties make the tensor class suitable for deep learning. Throughout the book, when we say tensors, we are referring to instances of the tensor class unless otherwise stated.

2.1.1 Getting Started

In this section, we aim to get you up and running, equipping you with the basic math and numerical computing tools that you will build on as you progress through the book. Do not worry if you struggle to grok some of the mathematical concepts or library functions. The following sections will revisit this material in the context of practical examples and it will sink in. On the other hand, if you already have some background and want to go deeper into the mathematical content, just skip this section.

To start, we import the np (numpy) and npx (numpy_extension) modules from MXNet. Here, the np module includes functions supported by NumPy, while the npx module contains a set of extensions developed to empower deep learning within a NumPy-like environment. When using tensors, we almost always invoke the set_np function: this is for compatibility of tensor processing by other components of MXNet.

```
from mxnet import np, npx  
  
npx.set_np()
```

A tensor represents a (possibly multi-dimensional) array of numerical values. With one axis, a tensor corresponds (in math) to a *vector*. With two axes, a tensor corresponds to a *matrix*. Tensors with more than two axes do not have special mathematical names.

To start, we can use arange to create a row vector x containing the first 12 integers starting with 0, though they are created as floats by default. Each of the values in a tensor is called an *element* of the tensor. For instance, there are 12 elements in the tensor x. Unless otherwise specified, a new tensor will be stored in main memory and designated for CPU-based computation.

```
x = np.arange(12)  
x  
  
array([ 0.,  1.,  2.,  3.,  4.,  5.,  6.,  7.,  8.,  9., 10., 11.])
```

We can access a tensor's *shape* (the length along each axis) by inspecting its shape property.

```
x.shape  
  
(12,)
```

If we just want to know the total number of elements in a tensor, i.e., the product of all of the shape elements, we can inspect its size. Because we are dealing with a vector here, the single element of its shape is identical to its size.

```
x.size
```

To change the shape of a tensor without altering either the number of elements or their values, we can invoke the `reshape` function. For example, we can transform our tensor, `x`, from a row vector with shape `(12,)` to a matrix with shape `(3, 4)`. This new tensor contains the exact same values, but views them as a matrix organized as 3 rows and 4 columns. To reiterate, although the shape has changed, the elements have not. Note that the size is unaltered by reshaping.

```
X = x.reshape(3, 4)
X
```

```
array([[ 0.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.]])
```

Reshaping by manually specifying every dimension is unnecessary. If our target shape is a matrix with shape `(height, width)`, then after we know the width, the height is given implicitly. Why should we have to perform the division ourselves? In the example above, to get a matrix with 3 rows, we specified both that it should have 3 rows and 4 columns. Fortunately, tensors can automatically work out one dimension given the rest. We invoke this capability by placing `-1` for the dimension that we would like tensors to automatically infer. In our case, instead of calling `x.reshape(3, 4)`, we could have equivalently called `x.reshape(-1, 4)` or `x.reshape(3, -1)`.

Typically, we will want our matrices initialized either with zeros, ones, some other constants, or numbers randomly sampled from a specific distribution. We can create a tensor representing a tensor with all elements set to 0 and a shape of `(2, 3, 4)` as follows:

```
np.zeros((2, 3, 4))
```

```
array([[[0., 0., 0., 0.],
       [0., 0., 0., 0.],
       [0., 0., 0., 0.]],

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

Similarly, we can create tensors with each element set to 1 as follows:

```
np.ones((2, 3, 4))
```

```
array([[[1., 1., 1., 1.],
       [1., 1., 1., 1.],
       [1., 1., 1., 1.]],

      [[1., 1., 1., 1.],
       [1., 1., 1., 1.],
       [1., 1., 1., 1.]]])
```

Often, we want to randomly sample the values for each element in a tensor from some probability distribution. For example, when we construct arrays to serve as parameters in a neural network,

we will typically initialize their values randomly. The following snippet creates a tensor with shape (3, 4). Each of its elements is randomly sampled from a standard Gaussian (normal) distribution with a mean of 0 and a standard deviation of 1.

```
np.random.normal(0, 1, size=(3, 4))
```

```
array([[ 2.2122064 ,  1.1630787 ,  0.7740038 ,  0.4838046 ],
       [ 1.0434405 ,  0.29956347,  1.1839255 ,  0.15302546],
       [ 1.8917114 , -1.1688148 , -1.2347414 ,  1.5580711 ]])
```

We can also specify the exact values for each element in the desired tensor by supplying a Python list (or list of lists) containing the numerical values. Here, the outermost list corresponds to axis 0, and the inner list to axis 1.

```
np.array([[2, 1, 4, 3], [1, 2, 3, 4], [4, 3, 2, 1]])
```

```
array([[2., 1., 4., 3.],
       [1., 2., 3., 4.],
       [4., 3., 2., 1.]])
```

2.1.2 Operations

This book is not about software engineering. Our interests are not limited to simply reading and writing data from/to arrays. We want to perform mathematical operations on those arrays. Some of the simplest and most useful operations are the *elementwise* operations. These apply a standard scalar operation to each element of an array. For functions that take two arrays as inputs, elementwise operations apply some standard binary operator on each pair of corresponding elements from the two arrays. We can create an elementwise function from any function that maps from a scalar to a scalar.

In mathematical notation, we would denote such a *unary* scalar operator (taking one input) by the signature $f : \mathbb{R} \rightarrow \mathbb{R}$. This just means that the function is mapping from any real number (\mathbb{R}) onto another. Likewise, we denote a *binary* scalar operator (taking two real inputs, and yielding one output) by the signature $f : \mathbb{R}, \mathbb{R} \rightarrow \mathbb{R}$. Given any two vectors \mathbf{u} and \mathbf{v} of *the same shape*, and a binary operator f , we can produce a vector $\mathbf{c} = F(\mathbf{u}, \mathbf{v})$ by setting $c_i \leftarrow f(u_i, v_i)$ for all i , where c_i , u_i , and v_i are the i^{th} elements of vectors \mathbf{c} , \mathbf{u} , and \mathbf{v} . Here, we produced the vector-valued $F : \mathbb{R}^d, \mathbb{R}^d \rightarrow \mathbb{R}^d$ by *lifting* the scalar function to an elementwise vector operation.

The common standard arithmetic operators (+, -, *, /, and **) have all been *lifted* to elementwise operations for any identically-shaped tensors of arbitrary shape. We can call elementwise operations on any two tensors of the same shape. In the following example, we use commas to formulate a 5-element tuple, where each element is the result of an elementwise operation.

Operations

The common standard arithmetic operators (+, -, *, /, and **) have all been *lifted* to elementwise operations.

```
x = np.array([1, 2, 4, 8])
y = np.array([2, 2, 2, 2])
x + y, x - y, x * y, x / y, x**y # The ** operator is exponentiation
```

```
(array([ 3.,  4.,  6., 10.]),
 array([-1.,  0.,  2.,  6.]),
 array([ 2.,  4.,  8., 16.]),
 array([0.5,  1. ,  2. ,  4. ]),
 array([ 1.,  4., 16., 64.]))
```

Many more operations can be applied elementwise, including unary operators like exponentiation.

```
np.exp(x)
```

```
array([2.7182817e+00, 7.3890562e+00, 5.4598148e+01, 2.9809580e+03])
```

In addition to elementwise computations, we can also perform linear algebra operations, including vector dot products and matrix multiplication. We will explain the crucial bits of linear algebra (with no assumed prior knowledge) in [Section 2.3](#).

We can also *concatenate* multiple tensors together, stacking them end-to-end to form a larger tensor. We just need to provide a list of tensors and tell the system along which axis to concatenate. The example below shows what happens when we concatenate two matrices along rows (axis 0, the first element of the shape) vs. columns (axis 1, the second element of the shape). We can see that the first output tensor's axis-0 length (6) is the sum of the two input tensors' axis-0 lengths (3 + 3); while the second output tensor's axis-1 length (8) is the sum of the two input tensors' axis-1 lengths (4 + 4).

```
X = np.arange(12).reshape(3, 4)
Y = np.array([[2, 1, 4, 3], [1, 2, 3, 4], [4, 3, 2, 1]])
np.concatenate([X, Y], axis=0), np.concatenate([X, Y], axis=1)
```

```
(array([[ 0.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.],
       [ 2.,  1.,  4.,  3.],
       [ 1.,  2.,  3.,  4.],
       [ 4.,  3.,  2.,  1.]]),
 array([[ 0.,  1.,  2.,  3.,  2.,  1.,  4.,  3.],
       [ 4.,  5.,  6.,  7.,  1.,  2.,  3.,  4.],
       [ 8.,  9., 10., 11.,  4.,  3.,  2.,  1.]]))
```

Sometimes, we want to construct a binary tensor via *logical statements*. Take `X == Y` as an example. For each position, if `X` and `Y` are equal at that position, the corresponding entry in the new tensor takes a value of 1, meaning that the logical statement `X == Y` is true at that position; otherwise that position takes 0.

```
X == Y
```

```
array([[False,  True, False,  True],
       [False, False, False, False],
       [False, False, False, False]])
```

Summing all the elements in the tensor yields a tensor with only one element.

```
X.sum()
```

```
array(66.)
```

2.1.3 Broadcasting Mechanism

In the above section, we saw how to perform elementwise operations on two tensors of the same shape. Under certain conditions, even when shapes differ, we can still perform elementwise operations by invoking the *broadcasting mechanism*. This mechanism works in the following way: First, expand one or both arrays by copying elements appropriately so that after this transformation, the two tensors have the same shape. Second, carry out the elementwise operations on the resulting arrays.

In most cases, we broadcast along an axis where an array initially only has length 1, such as in the following example:

```
a = np.arange(3).reshape(3, 1)
b = np.arange(2).reshape(1, 2)
a, b
```

```
(array([[0.],
       [1.],
       [2.]]),
 array([[0.,  1.]]))
```

Since `a` and `b` are 3×1 and 1×2 matrices respectively, their shapes do not match up if we want to add them. We *broadcast* the entries of both matrices into a larger 3×2 matrix as follows: for matrix `a` it replicates the columns and for matrix `b` it replicates the rows before adding up both elementwise.

```
a + b
```

```
array([[0.,  1.],
       [1.,  2.],
       [2.,  3.]])
```

2.1.4 Indexing and Slicing

Just as in any other Python array, elements in a tensor can be accessed by index. As in any Python array, the first element has index 0 and ranges are specified to include the first but *before* the last element. As in standard Python lists, we can access elements according to their relative position to the end of the list by using negative indices.

Thus, `[-1]` selects the last element and `[1:3]` selects the second and the third elements as follows:

```
X[-1], X[1:3]
```

```
(array([ 8.,  9., 10., 11.]),
 array([[ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.])))
```

Beyond reading, we can also write elements of a matrix by specifying indices.

```
X[1, 2] = 9
X
```

```
array([[ 0.,  1.,  2.,  3.],
       [ 4.,  5.,  9.,  7.],
       [ 8.,  9., 10., 11.]])
```

If we want to assign multiple elements the same value, we simply index all of them and then assign them the value. For instance, `[0:2, :]` accesses the first and second rows, where `:` takes all the elements along axis 1 (column). While we discussed indexing for matrices, this obviously also works for vectors and for tensors of more than 2 dimensions.

```
X[0:2, :] = 12
X
```

```
array([[12., 12., 12., 12.],
       [12., 12., 12., 12.],
       [ 8.,  9., 10., 11.]])
```

2.1.5 Saving Memory

Running operations can cause new memory to be allocated to host results. For example, if we write `Y = X + Y`, we will dereference the tensor that `Y` used to point to and instead point `Y` at the newly allocated memory. In the following example, we demonstrate this with Python's `id()` function, which gives us the exact address of the referenced object in memory. After running `Y = Y + X`, we will find that `id(Y)` points to a different location. That is because Python first evaluates `Y + X`, allocating new memory for the result and then makes `Y` point to this new location in memory.

```
before = id(Y)
Y = Y + X
id(Y) == before
```

```
False
```

This might be undesirable for two reasons. First, we do not want to run around allocating memory unnecessarily all the time. In machine learning, we might have hundreds of megabytes of parameters and update all of them multiple times per second. Typically, we will want to perform these updates *in place*. Second, we might point at the same parameters from multiple variables. If we do not update *in place*, other references will still point to the old memory location, making it possible for parts of our code to inadvertently reference stale parameters.

Fortunately, performing *in-place* operations is easy. We can assign the result of an operation to a previously allocated array with slice notation, e.g., $Y[:] = \text{<expression>}$. To illustrate this concept, we first create a new matrix Z with the same shape as another Y , using `zeros_like` to allocate a block of 0 entries.

```
Z = np.zeros_like(Y)
print('id(Z):', id(Z))
Z[:] = X + Y
print('id(Z):', id(Z))
```

```
id(Z): 140221399309824
id(Z): 140221399309824
```

If the value of X is not reused in subsequent computations, we can also use $X[:] = X + Y$ or $X += Y$ to reduce the memory overhead of the operation.

```
before = id(X)
X += Y
id(X) == before
```

```
True
```

2.1.6 Conversion to Other Python Objects

Converting to a NumPy tensor, or vice versa, is easy. The converted result does not share memory. This minor inconvenience is actually quite important: when you perform operations on the CPU or on GPUs, you do not want to halt computation, waiting to see whether the NumPy package of Python might want to be doing something else with the same chunk of memory.

```
A = X.asnumpy()
B = np.array(A)
type(A), type(B)
```

```
(numpy.ndarray, mxnet.numpy.ndarray)
```

To convert a size-1 tensor to a Python scalar, we can invoke the `item` function or Python's built-in functions.

```
a = np.array([3.5])
a, a.item(), float(a), int(a)
```

```
(array([3.5]), 3.5, 3.5, 3)
```

Summary

- The main interface to store and manipulate data for deep learning is the tensor (n -dimensional array). It provides a variety of functionalities including basic mathematics operations, broadcasting, indexing, slicing, memory saving, and conversion to other Python objects.

Exercises

1. Run the code in this section. Change the conditional statement $X == Y$ in this section to $X < Y$ or $X > Y$, and then see what kind of tensor you can get.
2. Replace the two tensors that operate by element in the broadcasting mechanism with other shapes, e.g., 3-dimensional tensors. Is the result the same as expected?

Discussions³⁹

2.2 Data Preprocessing

So far we have introduced a variety of techniques for manipulating data that are already stored in tensors. To apply deep learning to solving real-world problems, we often begin with preprocessing raw data, rather than those nicely prepared data in the tensor format. Among popular data analytic tools in Python, the pandas package is commonly used. Like many other extension packages in the vast ecosystem of Python, pandas can work together with tensors. So, we will briefly walk through steps for preprocessing raw data with pandas and converting them into the tensor format. We will cover more data preprocessing techniques in later chapters.

2.2.1 Reading the Dataset

As an example, we begin by creating an artificial dataset that is stored in a csv (comma-separated values) file `../data/house_tiny.csv`. Data stored in other formats may be processed in similar ways.

Below we write the dataset row by row into a csv file.

```
import os

os.makedirs(os.path.join('..', 'data'), exist_ok=True)
data_file = os.path.join('..', 'data', 'house_tiny.csv')
with open(data_file, 'w') as f:
    f.write('NumRooms,Alley,Price\n') # Column names
    f.write('NA,Pave,127500\n') # Each row represents a data example
    f.write('2,NA,106000\n')
    f.write('4,NA,178100\n')
    f.write('NA,NA,140000\n')
```

³⁹ <https://discuss.d2l.ai/t/26>

To load the raw dataset from the created csv file, we import the pandas package and invoke the `read_csv` function. This dataset has four rows and three columns, where each row describes the number of rooms (“NumRooms”), the alley type (“Alley”), and the price (“Price”) of a house.

```
# If pandas is not installed, just uncomment the following line:  
# !pip install pandas  
import pandas as pd  
  
data = pd.read_csv(data_file)  
print(data)
```

	NumRooms	Alley	Price
0	NaN	Pave	127500
1	2.0	NaN	106000
2	4.0	NaN	178100
3	NaN	NaN	140000

2.2.2 Handling Missing Data

Note that “NaN” entries are missing values. To handle missing data, typical methods include *imputation* and *deletion*, where imputation replaces missing values with substituted ones, while deletion ignores missing values. Here we will consider imputation.

By integer-location based indexing (`iloc`), we split data into inputs and outputs, where the former takes the first two columns while the latter only keeps the last column. For numerical values in inputs that are missing, we replace the “NaN” entries with the mean value of the same column.

```
inputs, outputs = data.iloc[:, 0:2], data.iloc[:, 2]  
inputs = inputs.fillna(inputs.mean())  
print(inputs)
```

	NumRooms	Alley
0	3.0	Pave
1	2.0	NaN
2	4.0	NaN
3	3.0	NaN

For categorical or discrete values in inputs, we consider “NaN” as a category. Since the “Alley” column only takes two types of categorical values “Pave” and “NaN”, pandas can automatically convert this column to two columns “Alley_Pave” and “Alley_nan”. A row whose alley type is “Pave” will set values of “Alley_Pave” and “Alley_nan” to 1 and 0. A row with a missing alley type will set their values to 0 and 1.

```
inputs = pd.get_dummies(inputs, dummy_na=True)  
print(inputs)
```

	NumRooms	Alley_Pave	Alley_nan
0	3.0	1	0
1	2.0	0	1
2	4.0	0	1
3	3.0	0	1

2.2.3 Conversion to the Tensor Format

Now that all the entries in inputs and outputs are numerical, they can be converted to the tensor format. Once data are in this format, they can be further manipulated with those tensor functionalities that we have introduced in Section 2.1.

```
from mxnet import np

X, y = np.array(inputs.values), np.array(outputs.values)
X, y

(array([[3., 1., 0.],
       [2., 0., 1.],
       [4., 0., 1.],
       [3., 0., 1.]], dtype=float64),
array([127500, 106000, 178100, 140000], dtype=int64))
```

Summary

- Like many other extension packages in the vast ecosystem of Python, pandas can work together with tensors.
- Imputation and deletion can be used to handle missing data.

Exercises

Create a raw dataset with more rows and columns.

1. Delete the column with the most missing values.
2. Convert the preprocessed dataset to the tensor format.

Discussions⁴⁰

2.3 Linear Algebra

Now that you can store and manipulate data, let us briefly review the subset of basic linear algebra that you will need to understand and implement most of models covered in this book. Below, we introduce the basic mathematical objects, arithmetic, and operations in linear algebra, expressing each of them through mathematical notation and the corresponding implementation in code.

⁴⁰ <https://discuss.d2l.ai/t/28>

2.3.1 Scalars

If you never studied linear algebra or machine learning, then your past experience with math probably consisted of thinking about one number at a time. And, if you ever balanced a checkbook or even paid for dinner at a restaurant then you already know how to do basic things like adding and multiplying pairs of numbers. For example, the temperature in Palo Alto is 52 degrees Fahrenheit. Formally, we call values consisting of just one numerical quantity *scalars*. If you wanted to convert this value to Celsius (the metric system's more sensible temperature scale), you would evaluate the expression $c = \frac{5}{9}(f - 32)$, setting f to 52. In this equation, each of the terms—5, 9, and 32—are scalar values. The placeholders c and f are called *variables* and they represent unknown scalar values.

In this book, we adopt the mathematical notation where scalar variables are denoted by ordinary lower-cased letters (e.g., x , y , and z). We denote the space of all (continuous) *real-valued* scalars by \mathbb{R} . For expedience, we will punt on rigorous definitions of what precisely *space* is, but just remember for now that the expression $x \in \mathbb{R}$ is a formal way to say that x is a real-valued scalar. The symbol \in can be pronounced “in” and simply denotes membership in a set. Analogously, we could write $x, y \in \{0, 1\}$ to state that x and y are numbers whose value can only be 0 or 1.

A scalar is represented by a tensor with just one element. In the next snippet, we instantiate two scalars and perform some familiar arithmetic operations with them, namely addition, multiplication, division, and exponentiation.

```
from mxnet import np, npx

npx.set_np()

x = np.array(3.0)
y = np.array(2.0)

x + y, x * y, x / y, x**y
```



```
(array(5.), array(6.), array(1.5), array(9.))
```

2.3.2 Vectors

You can think of a vector as simply a list of scalar values. We call these values the *elements (entries or components)* of the vector. When our vectors represent examples from our dataset, their values hold some real-world significance. For example, if we were training a model to predict the risk that a loan defaults, we might associate each applicant with a vector whose components correspond to their income, length of employment, number of previous defaults, and other factors. If we were studying the risk of heart attacks hospital patients potentially face, we might represent each patient by a vector whose components capture their most recent vital signs, cholesterol levels, minutes of exercise per day, etc. In math notation, we will usually denote vectors as bold-faced, lower-cased letters (e.g., \mathbf{x} , \mathbf{y} , and \mathbf{z}).

We work with vectors via one-dimensional tensors. In general tensors can have arbitrary lengths, subject to the memory limits of your machine.

```
x = np.arange(4)
x
```

```
array([0., 1., 2., 3.])
```

We can refer to any element of a vector by using a subscript. For example, we can refer to the i^{th} element of \mathbf{x} by x_i . Note that the element x_i is a scalar, so we do not bold-face the font when referring to it. Extensive literature considers column vectors to be the default orientation of vectors, so does this book. In math, a vector \mathbf{x} can be written as

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad (2.3.1)$$

where x_1, \dots, x_n are elements of the vector. In code, we access any element by indexing into the tensor.

```
x[3]
```

```
array(3.)
```

Length, Dimensionality, and Shape

Let us revisit some concepts from [Section 2.1](#). A vector is just an array of numbers. And just as every array has a length, so does every vector. In math notation, if we want to say that a vector \mathbf{x} consists of n real-valued scalars, we can express this as $\mathbf{x} \in \mathbb{R}^n$. The length of a vector is commonly called the *dimension* of the vector.

As with an ordinary Python array, we can access the length of a tensor by calling Python's built-in `len()` function.

```
len(x)
```

```
4
```

When a tensor represents a vector (with precisely one axis), we can also access its length via the `.shape` attribute. The shape is a tuple that lists the length (dimensionality) along each axis of the tensor. For tensors with just one axis, the shape has just one element.

```
x.shape
```

```
(4,)
```

Note that the word "dimension" tends to get overloaded in these contexts and this tends to confuse people. To clarify, we use the dimensionality of a *vector* or an *axis* to refer to its length, i.e., the number of elements of a vector or an axis. However, we use the dimensionality of a tensor to refer to the number of axes that a tensor has. In this sense, the dimensionality of some axis of a tensor will be the length of that axis.

2.3.3 Matrices

Just as vectors generalize scalars from order zero to order one, matrices generalize vectors from order one to order two. Matrices, which we will typically denote with bold-faced, capital letters (e.g., \mathbf{X} , \mathbf{Y} , and \mathbf{Z}), are represented in code as tensors with two axes.

In math notation, we use $\mathbf{A} \in \mathbb{R}^{m \times n}$ to express that the matrix \mathbf{A} consists of m rows and n columns of real-valued scalars. Visually, we can illustrate any matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ as a table, where each element a_{ij} belongs to the i^{th} row and j^{th} column:

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}. \quad (2.3.2)$$

For any $\mathbf{A} \in \mathbb{R}^{m \times n}$, the shape of \mathbf{A} is (m, n) or $m \times n$. Specifically, when a matrix has the same number of rows and columns, its shape becomes a square; thus, it is called a *square matrix*.

We can create an $m \times n$ matrix by specifying a shape with two components m and n when calling any of our favorite functions for instantiating a tensor.

```
A = np.arange(20).reshape(5, 4)
A
```

```
array([[ 0.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.],
       [12., 13., 14., 15.],
       [16., 17., 18., 19.]])
```

We can access the scalar element a_{ij} of a matrix \mathbf{A} in (2.3.2) by specifying the indices for the row (i) and column (j), such as $[\mathbf{A}]_{ij}$. When the scalar elements of a matrix \mathbf{A} , such as in (2.3.2), are not given, we may simply use the lower-case letter of the matrix \mathbf{A} with the index subscript, a_{ij} , to refer to $[\mathbf{A}]_{ij}$. To keep notation simple, commas are inserted to separate indices only when necessary, such as $a_{2,3j}$ and $[\mathbf{A}]_{2i-1,3}$.

Sometimes, we want to flip the axes. When we exchange a matrix's rows and columns, the result is called the *transpose* of the matrix. Formally, we signify a matrix \mathbf{A} 's transpose by \mathbf{A}^\top and if $\mathbf{B} = \mathbf{A}^\top$, then $b_{ij} = a_{ji}$ for any i and j . Thus, the transpose of \mathbf{A} in (2.3.2) is a $n \times m$ matrix:

$$\mathbf{A}^\top = \begin{bmatrix} a_{11} & a_{21} & \dots & a_{m1} \\ a_{12} & a_{22} & \dots & a_{m2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1n} & a_{2n} & \dots & a_{mn} \end{bmatrix}. \quad (2.3.3)$$

Now we access a matrix's transpose in code.

```
A.T
```

```
array([[ 0.,  4.,  8., 12., 16.],
       [ 1.,  5.,  9., 13., 17.],
       [ 2.,  6., 10., 14., 18.],
       [ 3.,  7., 11., 15., 19.]])
```

As a special type of the square matrix, a *symmetric matrix* \mathbf{A} is equal to its transpose: $\mathbf{A} = \mathbf{A}^\top$. Here we define a symmetric matrix \mathbf{B} .

```
B = np.array([[1, 2, 3], [2, 0, 4], [3, 4, 5]])  
B
```

```
array([[1., 2., 3.],  
       [2., 0., 4.],  
       [3., 4., 5.]])
```

Now we compare \mathbf{B} with its transpose.

```
B == B.T
```

```
array([[ True,  True,  True],  
       [ True,  True,  True],  
       [ True,  True,  True]])
```

Matrices are useful data structures: they allow us to organize data that have different modalities of variation. For example, rows in our matrix might correspond to different houses (data examples), while columns might correspond to different attributes. This should sound familiar if you have ever used spreadsheet software or have read [Section 2.2](#). Thus, although the default orientation of a single vector is a column vector, in a matrix that represents a tabular dataset, it is more conventional to treat each data example as a row vector in the matrix. And, as we will see in later chapters, this convention will enable common deep learning practices. For example, along the outermost axis of a tensor, we can access or enumerate minibatches of data examples, or just data examples if no minibatch exists.

2.3.4 Tensors

Just as vectors generalize scalars, and matrices generalize vectors, we can build data structures with even more axes. Tensors (“tensors” in this subsection refer to algebraic objects) give us a generic way of describing n -dimensional arrays with an arbitrary number of axes. Vectors, for example, are first-order tensors, and matrices are second-order tensors. Tensors are denoted with capital letters of a special font face (e.g., X , Y , and Z) and their indexing mechanism (e.g., x_{ijk} and $[X]_{1,2i-1,3}$) is similar to that of matrices.

Tensors will become more important when we start working with images, which arrive as n -dimensional arrays with 3 axes corresponding to the height, width, and a *channel* axis for stacking the color channels (red, green, and blue). For now, we will skip over higher order tensors and focus on the basics.

```
X = np.arange(24).reshape(2, 3, 4)  
X
```

```
array([[[ 0.,  1.,  2.,  3.],  
       [ 4.,  5.,  6.,  7.],  
       [ 8.,  9., 10., 11.]],  
  
      [[12., 13., 14., 15.],
```

(continues on next page)

```
[16., 17., 18., 19.],
[20., 21., 22., 23.]])
```

2.3.5 Basic Properties of Tensor Arithmetic

Scalars, vectors, matrices, and tensors (“tensors” in this subsection refer to algebraic objects) of an arbitrary number of axes have some nice properties that often come in handy. For example, you might have noticed from the definition of an elementwise operation that any elementwise unary operation does not change the shape of its operand. Similarly, given any two tensors with the same shape, the result of any binary elementwise operation will be a tensor of that same shape. For example, adding two matrices of the same shape performs elementwise addition over these two matrices.

```
A = np.arange(20).reshape(5, 4)
B = A.copy() # Assign a copy of 'A' to 'B' by allocating new memory
A, A + B
```

```
(array([[ 0.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.],
       [12., 13., 14., 15.],
       [16., 17., 18., 19.]]),
 array([[ 0.,  2.,  4.,  6.],
       [ 8., 10., 12., 14.],
       [16., 18., 20., 22.],
       [24., 26., 28., 30.],
       [32., 34., 36., 38.]]))
```

Specifically, elementwise multiplication of two matrices is called their *Hadamard product* (math notation \odot). Consider matrix $\mathbf{B} \in \mathbb{R}^{m \times n}$ whose element of row i and column j is b_{ij} . The Hadamard product of matrices \mathbf{A} (defined in (2.3.2)) and \mathbf{B}

$$\mathbf{A} \odot \mathbf{B} = \begin{bmatrix} a_{11}b_{11} & a_{12}b_{12} & \dots & a_{1n}b_{1n} \\ a_{21}b_{21} & a_{22}b_{22} & \dots & a_{2n}b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}b_{m1} & a_{m2}b_{m2} & \dots & a_{mn}b_{mn} \end{bmatrix}. \quad (2.3.4)$$

```
A * B
```

```
array([[ 0.,  1.,  4.,  9.],
       [16., 25., 36., 49.],
       [64., 81., 100., 121.],
       [144., 169., 196., 225.],
       [256., 289., 324., 361.]]))
```

Multiplying or adding a tensor by a scalar also does not change the shape of the tensor, where each element of the operand tensor will be added or multiplied by the scalar.

```
a = 2
X = np.arange(24).reshape(2, 3, 4)
a + X, (a * X).shape
```

```
(array([[[ 2.,  3.,  4.,  5.],
       [ 6.,  7.,  8.,  9.],
       [10., 11., 12., 13.]],

      [[14., 15., 16., 17.],
       [18., 19., 20., 21.],
       [22., 23., 24., 25.]]]),
 (2, 3, 4))
```

2.3.6 Reduction

One useful operation that we can perform with arbitrary tensors is to calculate the sum of their elements. In mathematical notation, we express sums using the \sum symbol. To express the sum of the elements in a vector \mathbf{x} of length d , we write $\sum_{i=1}^d x_i$. In code, we can just call the function for calculating the sum.

```
x = np.arange(4)
x, x.sum()
```

```
(array([0., 1., 2., 3.]), array(6.))
```

We can express sums over the elements of tensors of arbitrary shape. For example, the sum of the elements of an $m \times n$ matrix \mathbf{A} could be written $\sum_{i=1}^m \sum_{j=1}^n a_{ij}$.

```
A.shape, A.sum()
```

```
((5, 4), array(190.))
```

By default, invoking the function for calculating the sum *reduces* a tensor along all its axes to a scalar. We can also specify the axes along which the tensor is reduced via summation. Take matrices as an example. To reduce the row dimension (axis 0) by summing up elements of all the rows, we specify `axis=0` when invoking the function. Since the input matrix reduces along axis 0 to generate the output vector, the dimension of axis 0 of the input is lost in the output shape.

```
A_sum_axis0 = A.sum(axis=0)
A_sum_axis0, A_sum_axis0.shape
```

```
(array([40., 45., 50., 55.]), (4,))
```

Specifying `axis=1` will reduce the column dimension (axis 1) by summing up elements of all the columns. Thus, the dimension of axis 1 of the input is lost in the output shape.

```
A_sum_axis1 = A.sum(axis=1)
A_sum_axis1, A_sum_axis1.shape
```

```
(array([ 6., 22., 38., 54., 70.]), (5,))
```

Reducing a matrix along both rows and columns via summation is equivalent to summing up all the elements of the matrix.

```
A.sum(axis=[0, 1]) # Same as `A.sum()`
```

```
array(190.)
```

A related quantity is the *mean*, which is also called the *average*. We calculate the mean by dividing the sum by the total number of elements. In code, we could just call the function for calculating the mean on tensors of arbitrary shape.

```
A.mean(), A.sum() / A.size
```

```
(array(9.5), array(9.5))
```

Likewise, the function for calculating the mean can also reduce a tensor along the specified axes.

```
A.mean(axis=0), A.sum(axis=0) / A.shape[0]
```

```
(array([ 8., 9., 10., 11.]), array([ 8., 9., 10., 11.]))
```

Non-Reduction Sum

However, sometimes it can be useful to keep the number of axes unchanged when invoking the function for calculating the sum or mean.

```
sum_A = A.sum(axis=1, keepdims=True)
sum_A
```

```
array([[ 6.],
       [22.],
       [38.],
       [54.],
       [70.]])
```

For instance, since `sum_A` still keeps its two axes after summing each row, we can divide `A` by `sum_A` with broadcasting.

```
A / sum_A
```

```
array([[0. , 0.16666667, 0.33333334, 0.5       ],
       [0.18181819, 0.22727273, 0.27272728, 0.3181818 ],
       [0.21052632, 0.23684211, 0.2631579 , 0.28947368],
       [0.22222222, 0.24074075, 0.25925925, 0.27777778 ],
       [0.22857143, 0.24285714, 0.25714287, 0.27142859]])
```

If we want to calculate the cumulative sum of elements of \mathbf{A} along some axis, say $\text{axis}=0$ (row by row), we can call the `cumsum` function. This function will not reduce the input tensor along any axis.

```
A.cumsum(axis=0)
```

```
array([[ 0.,  1.,  2.,  3.],
       [ 4.,  6.,  8., 10.],
       [12., 15., 18., 21.],
       [24., 28., 32., 36.],
       [40., 45., 50., 55.]])
```

2.3.7 Dot Products

So far, we have only performed elementwise operations, sums, and averages. And if this was all we could do, linear algebra probably would not deserve its own section. However, one of the most fundamental operations is the dot product. Given two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$, their *dot product* $\mathbf{x}^\top \mathbf{y}$ (or $\langle \mathbf{x}, \mathbf{y} \rangle$) is a sum over the products of the elements at the same position: $\mathbf{x}^\top \mathbf{y} = \sum_{i=1}^d x_i y_i$.

```
y = np.ones(4)
x, y, np.dot(x, y)
```

```
(array([0., 1., 2., 3.]), array([1., 1., 1., 1.]), array(6.))
```

Note that we can express the dot product of two vectors equivalently by performing an elementwise multiplication and then a sum:

```
np.sum(x * y)
```

```
array(6.)
```

Dot products are useful in a wide range of contexts. For example, given some set of values, denoted by a vector $\mathbf{x} \in \mathbb{R}^d$ and a set of weights denoted by $\mathbf{w} \in \mathbb{R}^d$, the weighted sum of the values in \mathbf{x} according to the weights \mathbf{w} could be expressed as the dot product $\mathbf{x}^\top \mathbf{w}$. When the weights are non-negative and sum to one (i.e., $(\sum_{i=1}^d w_i = 1)$), the dot product expresses a *weighted average*. After normalizing two vectors to have the unit length, the dot products express the cosine of the angle between them. We will formally introduce this notion of *length* later in this section.

2.3.8 Matrix-Vector Products

Now that we know how to calculate dot products, we can begin to understand *matrix-vector products*. Recall the matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ and the vector $\mathbf{x} \in \mathbb{R}^n$ defined and visualized in (2.3.2) and (2.3.1) respectively. Let us start off by visualizing the matrix \mathbf{A} in terms of its row vectors

$$\mathbf{A} = \begin{bmatrix} \mathbf{a}_1^\top \\ \mathbf{a}_2^\top \\ \vdots \\ \mathbf{a}_m^\top \end{bmatrix}, \quad (2.3.5)$$

where each $\mathbf{a}_i^\top \in \mathbb{R}^n$ is a row vector representing the i^{th} row of the matrix \mathbf{A} .

The matrix-vector product \mathbf{Ax} is simply a column vector of length m , whose i^{th} element is the dot product $\mathbf{a}_i^\top \mathbf{x}$:

$$\mathbf{Ax} = \begin{bmatrix} \mathbf{a}_1^\top \\ \mathbf{a}_2^\top \\ \vdots \\ \mathbf{a}_m^\top \end{bmatrix} \mathbf{x} = \begin{bmatrix} \mathbf{a}_1^\top \mathbf{x} \\ \mathbf{a}_2^\top \mathbf{x} \\ \vdots \\ \mathbf{a}_m^\top \mathbf{x} \end{bmatrix}. \quad (2.3.6)$$

We can think of multiplication by a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ as a transformation that projects vectors from \mathbb{R}^n to \mathbb{R}^m . These transformations turn out to be remarkably useful. For example, we can represent rotations as multiplications by a square matrix. As we will see in subsequent chapters, we can also use matrix-vector products to describe the most intensive calculations required when computing each layer in a neural network given the values of the previous layer.

Expressing matrix-vector products in code with tensors, we use the same dot function as for dot products. When we call `np.dot(A, x)` with a matrix A and a vector x , the matrix-vector product is performed. Note that the column dimension of A (its length along axis 1) must be the same as the dimension of x (its length).

```
A.shape, x.shape, np.dot(A, x)
```

```
((5, 4), (4,), array([ 14.,  38.,  62.,  86., 110.]))
```

2.3.9 Matrix-Matrix Multiplication

If you have gotten the hang of dot products and matrix-vector products, then *matrix-matrix multiplication* should be straightforward.

Say that we have two matrices $\mathbf{A} \in \mathbb{R}^{n \times k}$ and $\mathbf{B} \in \mathbb{R}^{k \times m}$:

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nk} \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1m} \\ b_{21} & b_{22} & \cdots & b_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ b_{k1} & b_{k2} & \cdots & b_{km} \end{bmatrix}. \quad (2.3.7)$$

Denote by $\mathbf{a}_i^\top \in \mathbb{R}^k$ the row vector representing the i^{th} row of the matrix \mathbf{A} , and let $\mathbf{b}_j \in \mathbb{R}^k$ be the column vector from the j^{th} column of the matrix \mathbf{B} . To produce the matrix product $\mathbf{C} = \mathbf{AB}$, it is easiest to think of \mathbf{A} in terms of its row vectors and \mathbf{B} in terms of its column vectors:

$$\mathbf{A} = \begin{bmatrix} \mathbf{a}_1^\top \\ \mathbf{a}_2^\top \\ \vdots \\ \mathbf{a}_n^\top \end{bmatrix}, \quad \mathbf{B} = [\mathbf{b}_1 \ \mathbf{b}_2 \ \cdots \ \mathbf{b}_m]. \quad (2.3.8)$$

Then the matrix product $\mathbf{C} \in \mathbb{R}^{n \times m}$ is produced as we simply compute each element c_{ij} as the dot product $\mathbf{a}_i^\top \mathbf{b}_j$:

$$\mathbf{C} = \mathbf{AB} = \begin{bmatrix} \mathbf{a}_1^\top \\ \mathbf{a}_2^\top \\ \vdots \\ \mathbf{a}_n^\top \end{bmatrix} [\mathbf{b}_1 \ \mathbf{b}_2 \ \cdots \ \mathbf{b}_m] = \begin{bmatrix} \mathbf{a}_1^\top \mathbf{b}_1 & \mathbf{a}_1^\top \mathbf{b}_2 & \cdots & \mathbf{a}_1^\top \mathbf{b}_m \\ \mathbf{a}_2^\top \mathbf{b}_1 & \mathbf{a}_2^\top \mathbf{b}_2 & \cdots & \mathbf{a}_2^\top \mathbf{b}_m \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{a}_n^\top \mathbf{b}_1 & \mathbf{a}_n^\top \mathbf{b}_2 & \cdots & \mathbf{a}_n^\top \mathbf{b}_m \end{bmatrix}. \quad (2.3.9)$$

We can think of the matrix-matrix multiplication \mathbf{AB} as simply performing m matrix-vector products and stitching the results together to form an $n \times m$ matrix. In the following snippet, we perform matrix multiplication on A and B . Here, A is a matrix with 5 rows and 4 columns, and B is a matrix with 4 rows and 3 columns. After multiplication, we obtain a matrix with 5 rows and 3 columns.

```
B = np.ones(shape=(4, 3))
np.dot(A, B)
```

```
array([[ 6.,  6.,  6.],
       [22., 22., 22.],
       [38., 38., 38.],
       [54., 54., 54.],
       [70., 70., 70.]])
```

Matrix-matrix multiplication can be simply called *matrix multiplication*, and should not be confused with the Hadamard product.

2.3.10 Norms

Some of the most useful operators in linear algebra are *norms*. Informally, the norm of a vector tells us how *big* a vector is. The notion of *size* under consideration here concerns not dimensionality but rather the magnitude of the components.

In linear algebra, a vector norm is a function f that maps a vector to a scalar, satisfying a handful of properties. Given any vector \mathbf{x} , the first property says that if we scale all the elements of a vector by a constant factor α , its norm also scales by the *absolute value* of the same constant factor:

$$f(\alpha\mathbf{x}) = |\alpha|f(\mathbf{x}). \quad (2.3.10)$$

The second property is the familiar triangle inequality:

$$f(\mathbf{x} + \mathbf{y}) \leq f(\mathbf{x}) + f(\mathbf{y}). \quad (2.3.11)$$

The third property simply says that the norm must be non-negative:

$$f(\mathbf{x}) \geq 0. \quad (2.3.12)$$

That makes sense, as in most contexts the smallest *size* for anything is 0. The final property requires that the smallest norm is achieved and only achieved by a vector consisting of all zeros.

$$\forall i, [\mathbf{x}]_i = 0 \Leftrightarrow f(\mathbf{x}) = 0. \quad (2.3.13)$$

You might notice that norms sound a lot like measures of distance. And if you remember Euclidean distances (think Pythagoras' theorem) from grade school, then the concepts of non-negativity and the triangle inequality might ring a bell. In fact, the Euclidean distance is a norm: specifically it is the L_2 norm. Suppose that the elements in the n -dimensional vector \mathbf{x} are x_1, \dots, x_n .

The L_2 norm of \mathbf{x} is the square root of the sum of the squares of the vector elements:

$$\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^n x_i^2}, \quad (2.3.14)$$

where the subscript 2 is often omitted in L_2 norms, i.e., $\|\mathbf{x}\|$ is equivalent to $\|\mathbf{x}\|_2$. In code, we can calculate the L_2 norm of a vector as follows.

```
u = np.array([3, -4])
np.linalg.norm(u)
```

```
array(5.)
```

In deep learning, we work more often with the squared L_2 norm.

You will also frequently encounter the L_1 norm, which is expressed as the sum of the absolute values of the vector elements:

$$\|\mathbf{x}\|_1 = \sum_{i=1}^n |x_i|. \quad (2.3.15)$$

As compared with the L_2 norm, it is less influenced by outliers. To calculate the L_1 norm, we compose the absolute value function with a sum over the elements.

```
np.abs(u).sum()
```

```
array(7.)
```

Both the L_2 norm and the L_1 norm are special cases of the more general L_p norm:

$$\|\mathbf{x}\|_p = \left(\sum_{i=1}^n |x_i|^p \right)^{1/p}. \quad (2.3.16)$$

Analogous to L_2 norms of vectors, the *Frobenius norm* of a matrix $\mathbf{X} \in \mathbb{R}^{m \times n}$ is the square root of the sum of the squares of the matrix elements:

$$\|\mathbf{X}\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n x_{ij}^2}. \quad (2.3.17)$$

The Frobenius norm satisfies all the properties of vector norms. It behaves as if it were an L_2 norm of a matrix-shaped vector. Invoking the following function will calculate the Frobenius norm of a matrix.

```
np.linalg.norm(np.ones((4, 9)))
```

```
array(6.)
```

Norms and Objectives

While we do not want to get too far ahead of ourselves, we can plant some intuition already about why these concepts are useful. In deep learning, we are often trying to solve optimization problems: *maximize* the probability assigned to observed data; *minimize* the distance between predictions and the ground-truth observations. Assign vector representations to items (like words, products, or news articles) such that the distance between similar items is minimized, and the distance between dissimilar items is maximized. Oftentimes, the objectives, perhaps the most important components of deep learning algorithms (besides the data), are expressed as norms.

2.3.11 More on Linear Algebra

In just this section, we have taught you all the linear algebra that you will need to understand a remarkable chunk of modern deep learning. There is a lot more to linear algebra and a lot of that mathematics is useful for machine learning. For example, matrices can be decomposed into factors, and these decompositions can reveal low-dimensional structure in real-world datasets. There are entire subfields of machine learning that focus on using matrix decompositions and their generalizations to high-order tensors to discover structure in datasets and solve prediction problems. But this book focuses on deep learning. And we believe you will be much more inclined to learn more mathematics once you have gotten your hands dirty deploying useful machine learning models on real datasets. So while we reserve the right to introduce more mathematics much later on, we will wrap up this section here.

If you are eager to learn more about linear algebra, you may refer to either the [online appendix on linear algebraic operations⁴¹](#) or other excellent resources ([Strang, 1993](#); [Kolter, 2008](#); [Petersen et al., 2008](#)).

Summary

- Scalars, vectors, matrices, and tensors are basic mathematical objects in linear algebra.
- Vectors generalize scalars, and matrices generalize vectors.
- Scalars, vectors, matrices, and tensors have zero, one, two, and an arbitrary number of axes, respectively.
- A tensor can be reduced along the specified axes by `sum` and `mean`.
- Elementwise multiplication of two matrices is called their Hadamard product. It is different from matrix multiplication.
- In deep learning, we often work with norms such as the L_1 norm, the L_2 norm, and the Frobenius norm.
- We can perform a variety of operations over scalars, vectors, matrices, and tensors.

Exercises

1. Prove that the transpose of a matrix \mathbf{A} 's transpose is \mathbf{A} : $(\mathbf{A}^\top)^\top = \mathbf{A}$.
2. Given two matrices \mathbf{A} and \mathbf{B} , show that the sum of transposes is equal to the transpose of a sum: $\mathbf{A}^\top + \mathbf{B}^\top = (\mathbf{A} + \mathbf{B})^\top$.
3. Given any square matrix \mathbf{A} , is $\mathbf{A} + \mathbf{A}^\top$ always symmetric? Why?
4. We defined the tensor X of shape $(2, 3, 4)$ in this section. What is the output of `len(X)`?
5. For a tensor X of arbitrary shape, does `len(X)` always correspond to the length of a certain axis of X ? What is that axis?
6. Run `A / A.sum(axis=1)` and see what happens. Can you analyze the reason?
7. When traveling between two points in Manhattan, what is the distance that you need to cover in terms of the coordinates, i.e., in terms of avenues and streets? Can you travel diagonally?

⁴¹ https://d2l.ai/chapter_appendix-mathematics-for-deep-learning/geometry-linear-algebraic-ops.html

8. Consider a tensor with shape $(2, 3, 4)$. What are the shapes of the summation outputs along axis 0, 1, and 2?
9. Feed a tensor with 3 or more axes to the `linalg.norm` function and observe its output. What does this function compute for tensors of arbitrary shape?

Discussions⁴²

2.4 Calculus

Finding the area of a polygon had remained mysterious until at least 2,500 years ago, when ancient Greeks divided a polygon into triangles and summed their areas. To find the area of curved shapes, such as a circle, ancient Greeks inscribed polygons in such shapes. As shown in Fig. 2.4.1, an inscribed polygon with more sides of equal length better approximates the circle. This process is also known as the *method of exhaustion*.

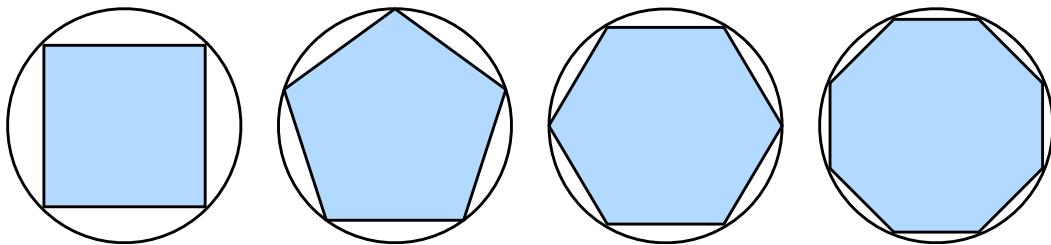


Fig. 2.4.1: Find the area of a circle with the method of exhaustion.

In fact, the method of exhaustion is where *integral calculus* (will be described in Section 18.5) originates from. More than 2,000 years later, the other branch of calculus, *differential calculus*, was invented. Among the most critical applications of differential calculus, optimization problems consider how to do something *the best*. As discussed in Section 2.3.10, such problems are ubiquitous in deep learning.

In deep learning, we *train* models, updating them successively so that they get better and better as they see more and more data. Usually, getting better means minimizing a *loss function*, a score that answers the question “how *bad* is our model?” This question is more subtle than it appears. Ultimately, what we really care about is producing a model that performs well on data that we have never seen before. But we can only fit the model to data that we can actually see. Thus we can decompose the task of fitting models into two key concerns: i) *optimization*: the process of fitting our models to observed data; ii) *generalization*: the mathematical principles and practitioners’ wisdom that guide as to how to produce models whose validity extends beyond the exact set of data examples used to train them.

To help you understand optimization problems and methods in later chapters, here we give a very brief primer on differential calculus that is commonly used in deep learning.

⁴² <https://discuss.d2l.ai/t/30>

2.4.1 Derivatives and Differentiation

We begin by addressing the calculation of derivatives, a crucial step in nearly all deep learning optimization algorithms. In deep learning, we typically choose loss functions that are differentiable with respect to our model's parameters. Put simply, this means that for each parameter, we can determine how rapidly the loss would increase or decrease, were we to *increase* or *decrease* that parameter by an infinitesimally small amount.

Suppose that we have a function $f : \mathbb{R} \rightarrow \mathbb{R}$, whose input and output are both scalars. The *derivative* of f is defined as

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}, \quad (2.4.1)$$

if this limit exists. If $f'(a)$ exists, f is said to be *differentiable* at a . If f is differentiable at every number of an interval, then this function is differentiable on this interval. We can interpret the derivative $f'(x)$ in (2.4.1) as the *instantaneous* rate of change of $f(x)$ with respect to x . The so-called instantaneous rate of change is based on the variation h in x , which approaches 0.

To illustrate derivatives, let us experiment with an example. Define $u = f(x) = 3x^2 - 4x$.

```
%matplotlib inline
from IPython import display
from mxnet import np, npx
from d2l import mxnet as d2l

npx.set_np()

def f(x):
    return 3 * x ** 2 - 4 * x
```

By setting $x = 1$ and letting h approach 0, the numerical result of $\frac{f(x+h)-f(x)}{h}$ in (2.4.1) approaches 2. Though this experiment is not a mathematical proof, we will see later that the derivative u' is 2 when $x = 1$.

```
def numerical_lim(f, x, h):
    return (f(x + h) - f(x)) / h

h = 0.1
for i in range(5):
    print(f'h={h:.5f}, numerical limit={numerical_lim(f, 1, h):.5f}')
    h *= 0.1
```

```
h=0.10000, numerical limit=2.30000
h=0.01000, numerical limit=2.03000
h=0.00100, numerical limit=2.00300
h=0.00010, numerical limit=2.00030
h=0.00001, numerical limit=2.00003
```

Let us familiarize ourselves with a few equivalent notations for derivatives. Given $y = f(x)$, where x and y are the independent variable and the dependent variable of the function f , respectively. The following expressions are equivalent:

$$f'(x) = y' = \frac{dy}{dx} = \frac{df}{dx} = \frac{d}{dx} f(x) = Df(x) = D_x f(x), \quad (2.4.2)$$

where symbols $\frac{d}{dx}$ and D are *differentiation operators* that indicate operation of *differentiation*. We can use the following rules to differentiate common functions:

- $DC = 0$ (C is a constant),
- $Dx^n = nx^{n-1}$ (the *power rule*, n is any real number),
- $De^x = e^x$,
- $D \ln(x) = 1/x$.

To differentiate a function that is formed from a few simpler functions such as the above common functions, the following rules can be handy for us. Suppose that functions f and g are both differentiable and C is a constant, we have the *constant multiple rule*

$$\frac{d}{dx}[Cf(x)] = C\frac{d}{dx}f(x), \quad (2.4.3)$$

the *sum rule*

$$\frac{d}{dx}[f(x) + g(x)] = \frac{d}{dx}f(x) + \frac{d}{dx}g(x), \quad (2.4.4)$$

the *product rule*

$$\frac{d}{dx}[f(x)g(x)] = f(x)\frac{d}{dx}[g(x)] + g(x)\frac{d}{dx}[f(x)], \quad (2.4.5)$$

and the *quotient rule*

$$\frac{d}{dx}\left[\frac{f(x)}{g(x)}\right] = \frac{g(x)\frac{d}{dx}[f(x)] - f(x)\frac{d}{dx}[g(x)]}{[g(x)]^2}. \quad (2.4.6)$$

Now we can apply a few of the above rules to find $u' = f'(x) = 3\frac{d}{dx}x^2 - 4\frac{d}{dx}x = 6x - 4$. Thus, by setting $x = 1$, we have $u' = 2$: this is supported by our earlier experiment in this section where the numerical result approaches 2. This derivative is also the slope of the tangent line to the curve $u = f(x)$ when $x = 1$.

To visualize such an interpretation of derivatives, we will use `matplotlib`, a popular plotting library in Python. To configure properties of the figures produced by `matplotlib`, we need to define a few functions. In the following, the `use_svg_display` function specifies the `matplotlib` package to output the `svg` figures for sharper images. Note that the comment `#@save` is a special mark where the following function, class, or statements are saved in the `d2l` package so later they can be directly invoked (e.g., `d2l.use_svg_display()`) without being redefined.

```
def use_svg_display():  #@save
    """Use the svg format to display a plot in Jupyter."""
    display.set_matplotlib_formats('svg')
```

We define the `set_figsize` function to specify the figure sizes. Note that here we directly use `d2l.plt` since the import statement from `matplotlib import pyplot as plt` has been marked for being saved in the `d2l` package in the preface.

```
def set_figsize(figsize=(3.5, 2.5)):  #@save
    """Set the figure size for matplotlib."""
    use_svg_display()
    d2l.plt.rcParams['figure.figsize'] = figsize
```

The following `set_axes` function sets properties of axes of figures produced by `matplotlib`.

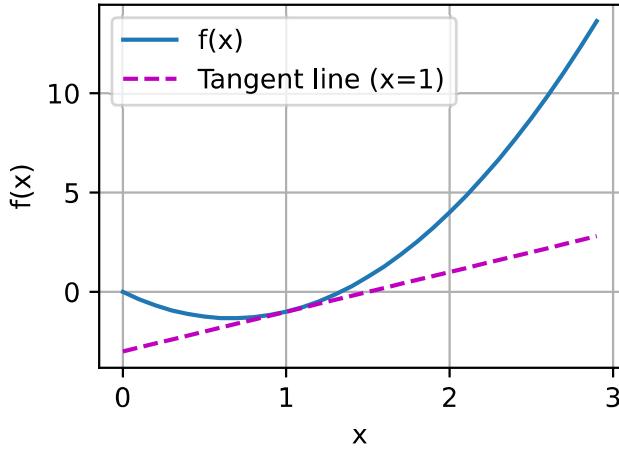
```
#@save
def set_axes(axes, xlabel, ylabel, xlim, ylim, xscale, yscale, legend):
    """Set the axes for matplotlib."""
    axes.set_xlabel(xlabel)
    axes.set_ylabel(ylabel)
    axes.set_xscale(xscale)
    axes.set_yscale(yscale)
    axes.set_xlim(xlim)
    axes.set_ylim(ylim)
    if legend:
        axes.legend(legend)
    axes.grid()
```

With these three functions for figure configurations, we define the `plot` function to plot multiple curves succinctly since we will need to visualize many curves throughout the book.

```
#@save
def plot(X, Y=None, xlabel=None, ylabel=None, legend=None, xlim=None,
         ylim=None, xscale='linear', yscale='linear',
         fmts=('-', 'm--', 'g-.', 'r:'), figsize=(3.5, 2.5), axes=None):
    """Plot data points."""
    if legend is None:
        legend = []
    set_figsize(figsize)
    axes = axes if axes else d2l.plt.gca()
    # Return True if 'X' (tensor or list) has 1 axis
    def has_one_axis(X):
        return (hasattr(X, "ndim") and X.ndim == 1 or
               isinstance(X, list) and not hasattr(X[0], "__len__"))
    if has_one_axis(X):
        X = [X]
    if Y is None:
        X, Y = [[[]]] * len(X), X
    elif has_one_axis(Y):
        Y = [Y]
    if len(X) != len(Y):
        X = X * len(Y)
    axes.cla()
    for x, y, fmt in zip(X, Y, fmts):
        if len(x):
            axes.plot(x, y, fmt)
        else:
            axes.plot(y, fmt)
    set_axes(axes, xlabel, ylabel, xlim, ylim, xscale, yscale, legend)
```

Now we can plot the function $u = f(x)$ and its tangent line $y = 2x - 3$ at $x = 1$, where the coefficient 2 is the slope of the tangent line.

```
x = np.arange(0, 3, 0.1)
plot(x, [f(x), 2 * x - 3], 'x', 'f(x)', legend=['f(x)', 'Tangent line (x=1)'])
```



2.4.2 Partial Derivatives

So far we have dealt with the differentiation of functions of just one variable. In deep learning, functions often depend on *many* variables. Thus, we need to extend the ideas of differentiation to these *multivariate* functions.

Let $y = f(x_1, x_2, \dots, x_n)$ be a function with n variables. The *partial derivative* of y with respect to its i^{th} parameter x_i is

$$\frac{\partial y}{\partial x_i} = \lim_{h \rightarrow 0} \frac{f(x_1, \dots, x_{i-1}, x_i + h, x_{i+1}, \dots, x_n) - f(x_1, \dots, x_i, \dots, x_n)}{h}. \quad (2.4.7)$$

To calculate $\frac{\partial y}{\partial x_i}$, we can simply treat $x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n$ as constants and calculate the derivative of y with respect to x_i . For notation of partial derivatives, the following are equivalent:

$$\frac{\partial y}{\partial x_i} = \frac{\partial f}{\partial x_i} = f_{x_i} = f_i = D_i f = D_{x_i} f. \quad (2.4.8)$$

2.4.3 Gradients

We can concatenate partial derivatives of a multivariate function with respect to all its variables to obtain the *gradient* vector of the function. Suppose that the input of function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is an n -dimensional vector $\mathbf{x} = [x_1, x_2, \dots, x_n]^\top$ and the output is a scalar. The gradient of the function $f(\mathbf{x})$ with respect to \mathbf{x} is a vector of n partial derivatives:

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \left[\frac{\partial f(\mathbf{x})}{\partial x_1}, \frac{\partial f(\mathbf{x})}{\partial x_2}, \dots, \frac{\partial f(\mathbf{x})}{\partial x_n} \right]^\top, \quad (2.4.9)$$

where $\nabla_{\mathbf{x}} f(\mathbf{x})$ is often replaced by $\nabla f(\mathbf{x})$ when there is no ambiguity.

Let \mathbf{x} be an n -dimensional vector, the following rules are often used when differentiating multivariate functions:

- For all $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\nabla_{\mathbf{x}} \mathbf{A}\mathbf{x} = \mathbf{A}^\top$,
- For all $\mathbf{A} \in \mathbb{R}^{n \times m}$, $\nabla_{\mathbf{x}} \mathbf{x}^\top \mathbf{A} = \mathbf{A}$,
- For all $\mathbf{A} \in \mathbb{R}^{n \times n}$, $\nabla_{\mathbf{x}} \mathbf{x}^\top \mathbf{A}\mathbf{x} = (\mathbf{A} + \mathbf{A}^\top)\mathbf{x}$,
- $\nabla_{\mathbf{x}} \|\mathbf{x}\|^2 = \nabla_{\mathbf{x}} \mathbf{x}^\top \mathbf{x} = 2\mathbf{x}$.

Similarly, for any matrix \mathbf{X} , we have $\nabla_{\mathbf{X}} \|\mathbf{X}\|_F^2 = 2\mathbf{X}$. As we will see later, gradients are useful for designing optimization algorithms in deep learning.

2.4.4 Chain Rule

However, such gradients can be hard to find. This is because multivariate functions in deep learning are often *composite*, so we may not apply any of the aforementioned rules to differentiate these functions. Fortunately, the *chain rule* enables us to differentiate composite functions.

Let us first consider functions of a single variable. Suppose that functions $y = f(u)$ and $u = g(x)$ are both differentiable, then the chain rule states that

$$\frac{dy}{dx} = \frac{dy}{du} \frac{du}{dx}. \quad (2.4.10)$$

Now let us turn our attention to a more general scenario where functions have an arbitrary number of variables. Suppose that the differentiable function y has variables u_1, u_2, \dots, u_m , where each differentiable function u_i has variables x_1, x_2, \dots, x_n . Note that y is a function of x_1, x_2, \dots, x_n . Then the chain rule gives

$$\frac{dy}{dx_i} = \frac{dy}{du_1} \frac{du_1}{dx_i} + \frac{dy}{du_2} \frac{du_2}{dx_i} + \dots + \frac{dy}{du_m} \frac{du_m}{dx_i} \quad (2.4.11)$$

for any $i = 1, 2, \dots, n$.

Summary

- Differential calculus and integral calculus are two branches of calculus, where the former can be applied to the ubiquitous optimization problems in deep learning.
- A derivative can be interpreted as the instantaneous rate of change of a function with respect to its variable. It is also the slope of the tangent line to the curve of the function.
- A gradient is a vector whose components are the partial derivatives of a multivariate function with respect to all its variables.
- The chain rule enables us to differentiate composite functions.

Exercises

1. Plot the function $y = f(x) = x^3 - \frac{1}{x}$ and its tangent line when $x = 1$.
2. Find the gradient of the function $f(\mathbf{x}) = 3x_1^2 + 5e^{x_2}$.
3. What is the gradient of the function $f(\mathbf{x}) = \|\mathbf{x}\|_2$?
4. Can you write out the chain rule for the case where $u = f(x, y, z)$ and $x = x(a, b)$, $y = y(a, b)$, and $z = z(a, b)$?

Discussions⁴³

⁴³ <https://discuss.d2l.ai/t/32>

2.5 Automatic Differentiation

As we have explained in Section 2.4, differentiation is a crucial step in nearly all deep learning optimization algorithms. While the calculations for taking these derivatives are straightforward, requiring only some basic calculus, for complex models, working out the updates by hand can be a pain (and often error-prone).

Deep learning frameworks expedite this work by automatically calculating derivatives, i.e., *automatic differentiation*. In practice, based on our designed model the system builds a *computational graph*, tracking which data combined through which operations to produce the output. Automatic differentiation enables the system to subsequently backpropagate gradients. Here, *backpropagate* simply means to trace through the computational graph, filling in the partial derivatives with respect to each parameter.

2.5.1 A Simple Example

As a toy example, say that we are interested in differentiating the function $y = 2\mathbf{x}^\top \mathbf{x}$ with respect to the column vector \mathbf{x} . To start, let us create the variable \mathbf{x} and assign it an initial value.

```
from mxnet import autograd, np, npx

npx.set_np()

x = np.arange(4.0)
x
```

```
array([0., 1., 2., 3.])
```

Before we even calculate the gradient of y with respect to \mathbf{x} , we will need a place to store it. It is important that we do not allocate new memory every time we take a derivative with respect to a parameter because we will often update the same parameters thousands or millions of times and could quickly run out of memory. Note that a gradient of a scalar-valued function with respect to a vector \mathbf{x} is itself vector-valued and has the same shape as \mathbf{x} .

```
# We allocate memory for a tensor's gradient by invoking 'attach_grad'
x.attach_grad()
# After we calculate a gradient taken with respect to 'x', we will be able to
# access it via the 'grad' attribute, whose values are initialized with 0s
x.grad
```

```
array([0., 0., 0., 0.])
```

Now let us calculate y .

```
# Place our code inside an 'autograd.record' scope to build the computational
# graph
with autograd.record():
    y = 2 * np.dot(x, x)
y
```

```
array(28.)
```

Since x is a vector of length 4, an inner product of x and x is performed, yielding the scalar output that we assign to y . Next, we can automatically calculate the gradient of y with respect to each component of x by calling the function for backpropagation and printing the gradient.

```
y.backward()  
x.grad
```

```
array([ 0.,  4.,  8., 12.])
```

The gradient of the function $y = 2\mathbf{x}^\top \mathbf{x}$ with respect to \mathbf{x} should be $4\mathbf{x}$. Let us quickly verify that our desired gradient was calculated correctly.

```
x.grad == 4 * x
```

```
array([ True,  True,  True,  True])
```

Now let us calculate another function of x .

```
with autograd.record():  
    y = x.sum()  
y.backward()  
x.grad # Overwritten by the newly calculated gradient
```

```
array([1., 1., 1., 1.])
```

2.5.2 Backward for Non-Scalar Variables

Technically, when y is not a scalar, the most natural interpretation of the differentiation of a vector y with respect to a vector x is a matrix. For higher-order and higher-dimensional y and x , the differentiation result could be a high-order tensor.

However, while these more exotic objects do show up in advanced machine learning (including in deep learning), more often when we are calling `backward` on a vector, we are trying to calculate the derivatives of the loss functions for each constituent of a *batch* of training examples. Here, our intent is not to calculate the differentiation matrix but rather the sum of the partial derivatives computed individually for each example in the batch.

```
# When we invoke 'backward' on a vector-valued variable 'y' (function of 'x'),  
# a new scalar variable is created by summing the elements in 'y'. Then the  
# gradient of that scalar variable with respect to 'x' is computed  
with autograd.record():  
    y = x * x # 'y' is a vector  
y.backward()  
x.grad # Equals to y = sum(x * x)
```

```
array([0., 2., 4., 6.])
```

2.5.3 Detaching Computation

Sometimes, we wish to move some calculations outside of the recorded computational graph. For example, say that y was calculated as a function of x , and that subsequently z was calculated as a function of both y and x . Now, imagine that we wanted to calculate the gradient of z with respect to x , but wanted for some reason to treat y as a constant, and only take into account the role that x played after y was calculated.

Here, we can detach y to return a new variable u that has the same value as y but discards any information about how y was computed in the computational graph. In other words, the gradient will not flow backwards through u to x . Thus, the following backpropagation function computes the partial derivative of $z = u * x$ with respect to x while treating u as a constant, instead of the partial derivative of $z = x * x * x$ with respect to x .

```
with autograd.record():
    y = x * x
    u = y.detach()
    z = u * x
z.backward()
x.grad == u
```

```
array([ True,  True,  True,  True])
```

Since the computation of y was recorded, we can subsequently invoke backpropagation on y to get the derivative of $y = x * x$ with respect to x , which is $2 * x$.

```
y.backward()
x.grad == 2 * x
```

```
array([ True,  True,  True,  True])
```

2.5.4 Computing the Gradient of Python Control Flow

One benefit of using automatic differentiation is that even if building the computational graph of a function required passing through a maze of Python control flow (e.g., conditionals, loops, and arbitrary function calls), we can still calculate the gradient of the resulting variable. In the following snippet, note that the number of iterations of the while loop and the evaluation of the if statement both depend on the value of the input a .

```
def f(a):
    b = a * 2
    while np.linalg.norm(b) < 1000:
        b = b * 2
    if b.sum() > 0:
        c = b
    else:
        c = 100 * b
    return c
```

Let us compute the gradient.

```

a = np.random.normal()
a.attach_grad()
with autograd.record():
    d = f(a)
d.backward()

```

We can now analyze the `f` function defined above. Note that it is piecewise linear in its input `a`. In other words, for any `a` there exists some constant scalar `k` such that $f(a) = k * a$, where the value of `k` depends on the input `a`. Consequently `d / a` allows us to verify that the gradient is correct.

```
a.grad == d / a
```

```
array(True)
```

Summary

- Deep learning frameworks can automate the calculation of derivatives. To use it, we first attach gradients to those variables with respect to which we desire partial derivatives. We then record the computation of our target value, execute its function for backpropagation, and access the resulting gradient.

Exercises

1. Why is the second derivative much more expensive to compute than the first derivative?
2. After running the function for backpropagation, immediately run it again and see what happens.
3. In the control flow example where we calculate the derivative of `d` with respect to `a`, what would happen if we changed the variable `a` to a random vector or matrix. At this point, the result of the calculation `f(a)` is no longer a scalar. What happens to the result? How do we analyze this?
4. Redesign an example of finding the gradient of the control flow. Run and analyze the result.
5. Let $f(x) = \sin(x)$. Plot $f(x)$ and $\frac{df(x)}{dx}$, where the latter is computed without exploiting that $f'(x) = \cos(x)$.

Discussions⁴⁴

⁴⁴ <https://discuss.d2l.ai/t/34>

2.6 Probability

In some form or another, machine learning is all about making predictions. We might want to predict the *probability* of a patient suffering a heart attack in the next year, given their clinical history. In anomaly detection, we might want to assess how *likely* a set of readings from an airplane's jet engine would be, were it operating normally. In reinforcement learning, we want an agent to act intelligently in an environment. This means we need to think about the probability of getting a high reward under each of the available actions. And when we build recommender systems we also need to think about probability. For example, say *hypothetically* that we worked for a large online bookseller. We might want to estimate the probability that a particular user would buy a particular book. For this we need to use the language of probability. Entire courses, majors, theses, careers, and even departments, are devoted to probability. So naturally, our goal in this section is not to teach the whole subject. Instead we hope to get you off the ground, to teach you just enough that you can start building your first deep learning models, and to give you enough of a flavor for the subject that you can begin to explore it on your own if you wish.

We have already invoked probabilities in previous sections without articulating what precisely they are or giving a concrete example. Let us get more serious now by considering the first case: distinguishing cats and dogs based on photographs. This might sound simple but it is actually a formidable challenge. To start with, the difficulty of the problem may depend on the resolution of the image.



Fig. 2.6.1: Images of varying resolutions (10×10 , 20×20 , 40×40 , 80×80 , and 160×160 pixels).

As shown in Fig. 2.6.1, while it is easy for humans to recognize cats and dogs at the resolution of 160×160 pixels, it becomes challenging at 40×40 pixels and next to impossible at 10×10 pixels. In other words, our ability to tell cats and dogs apart at a large distance (and thus low resolution) might approach uninformed guessing. Probability gives us a formal way of reasoning about our level of certainty. If we are completely sure that the image depicts a cat, we say that the *probability* that the corresponding label y is “cat”, denoted $P(y = \text{“cat”})$ equals 1. If we had no evidence to suggest that $y = \text{“cat”}$ or that $y = \text{“dog”}$, then we might say that the two possibilities were equally *likely* expressing this as $P(y = \text{“cat”}) = P(y = \text{“dog”}) = 0.5$. If we were reasonably confident, but not sure that the image depicted a cat, we might assign a probability $0.5 < P(y = \text{“cat”}) < 1$.

Now consider the second case: given some weather monitoring data, we want to predict the probability that it will rain in Taipei tomorrow. If it is summertime, the rain might come with probability 0.5.

In both cases, we have some value of interest. And in both cases we are uncertain about the outcome. But there is a key difference between the two cases. In this first case, the image is in fact either a dog or a cat, and we just do not know which. In the second case, the outcome may actually be a random event, if you believe in such things (and most physicists do). So probability is a flexible language for reasoning about our level of certainty, and it can be applied effectively in a broad set of contexts.

2.6.1 Basic Probability Theory

Say that we cast a die and want to know what the chance is of seeing a 1 rather than another digit. If the die is fair, all the six outcomes $\{1, \dots, 6\}$ are equally likely to occur, and thus we would see a 1 in one out of six cases. Formally we state that 1 occurs with probability $\frac{1}{6}$.

For a real die that we receive from a factory, we might not know those proportions and we would need to check whether it is tainted. The only way to investigate the die is by casting it many times and recording the outcomes. For each cast of the die, we will observe a value in $\{1, \dots, 6\}$. Given these outcomes, we want to investigate the probability of observing each outcome.

One natural approach for each value is to take the individual count for that value and to divide it by the total number of tosses. This gives us an *estimate* of the probability of a given *event*. The *law of large numbers* tell us that as the number of tosses grows this estimate will draw closer and closer to the true underlying probability. Before going into the details of what is going here, let us try it out.

To start, let us import the necessary packages.

```
%matplotlib inline
import random
from mxnet import np, npx
from d2l import mxnet as d2l

npx.set_np()
```

Next, we will want to be able to cast the die. In statistics we call this process of drawing examples from probability distributions *sampling*. The distribution that assigns probabilities to a number of discrete choices is called the *multinomial distribution*. We will give a more formal definition of *distribution* later, but at a high level, think of it as just an assignment of probabilities to events.

To draw a single sample, we simply pass in a vector of probabilities. The output is another vector of the same length: its value at index i is the number of times the sampling outcome corresponds to i .

```
fair_probs = [1.0 / 6] * 6
np.random.multinomial(1, fair_probs)

array([0, 0, 0, 1, 0, 0], dtype=int64)
```

If you run the sampler a bunch of times, you will find that you get out random values each time. As with estimating the fairness of a die, we often want to generate many samples from the same

distribution. It would be unbearably slow to do this with a Python for loop, so the function we are using supports drawing multiple samples at once, returning an array of independent samples in any shape we might desire.

```
np.random.multinomial(10, fair_probs)
```

```
array([1, 1, 5, 1, 1, 1], dtype=int64)
```

Now that we know how to sample rolls of a die, we can simulate 1000 rolls. We can then go through and count, after each of the 1000 rolls, how many times each number was rolled. Specifically, we calculate the relative frequency as the estimate of the true probability.

```
counts = np.random.multinomial(1000, fair_probs).astype(np.float32)
counts / 1000
```

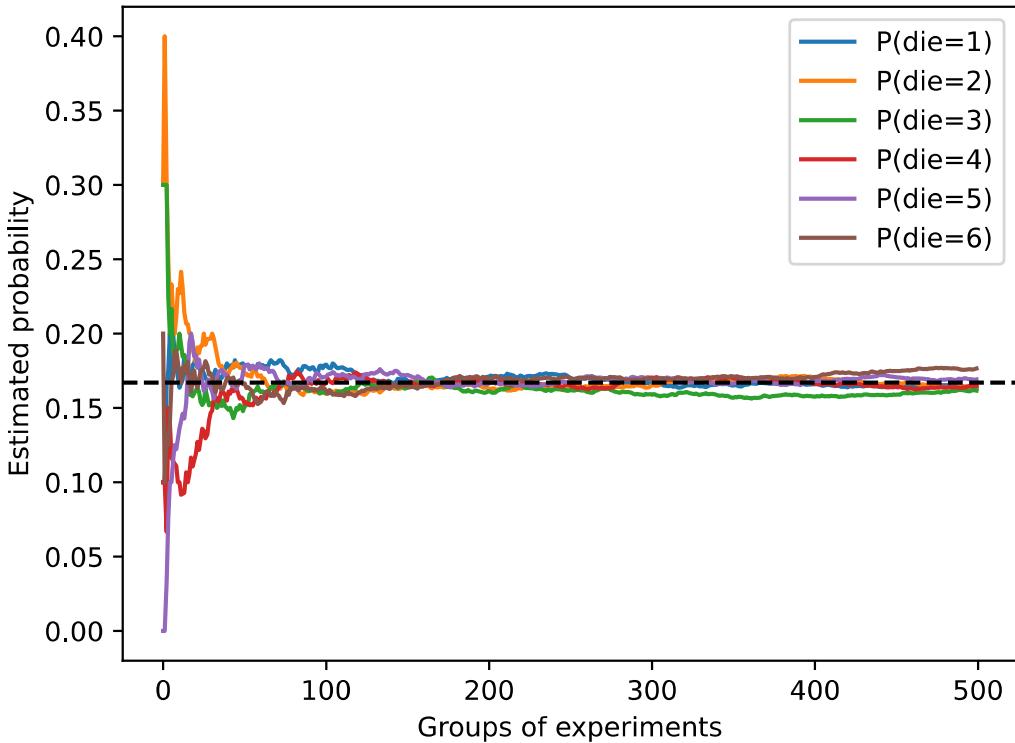
```
array([0.162, 0.149, 0.178, 0.17 , 0.166, 0.175])
```

Because we generated the data from a fair die, we know that each outcome has true probability $\frac{1}{6}$, roughly 0.167, so the above output estimates look good.

We can also visualize how these probabilities converge over time towards the true probability. Let us conduct 500 groups of experiments where each group draws 10 samples.

```
counts = np.random.multinomial(10, fair_probs, size=500)
cum_counts = counts.astype(np.float32).cumsum(axis=0)
estimates = cum_counts / cum_counts.sum(axis=1, keepdims=True)

d2l.set_figsize((6, 4.5))
for i in range(6):
    d2l.plt.plot(estimates[:, i].asnumpy(),
                  label=("P(die=" + str(i + 1) + ")"))
d2l.plt.axhline(y=0.167, color='black', linestyle='dashed')
d2l.plt.gca().set_xlabel('Groups of experiments')
d2l.plt.gca().set_ylabel('Estimated probability')
d2l.plt.legend();
```



Each solid curve corresponds to one of the six values of the die and gives our estimated probability that the die turns up that value as assessed after each group of experiments. The dashed black line gives the true underlying probability. As we get more data by conducting more experiments, the 6 solid curves converge towards the true probability.

Axioms of Probability Theory

When dealing with the rolls of a die, we call the set $\mathcal{S} = \{1, 2, 3, 4, 5, 6\}$ the *sample space* or *outcome space*, where each element is an *outcome*. An *event* is a set of outcomes from a given sample space. For instance, “seeing a 5” ($\{5\}$) and “seeing an odd number” ($\{1, 3, 5\}$) are both valid events of rolling a die. Note that if the outcome of a random experiment is in event \mathcal{A} , then event \mathcal{A} has occurred. That is to say, if 3 dots faced up after rolling a die, since $3 \in \{1, 3, 5\}$, we can say that the event “seeing an odd number” has occurred.

Formally, *probability* can be thought of as a function that maps a set to a real value. The probability of an event \mathcal{A} in the given sample space \mathcal{S} , denoted as $P(\mathcal{A})$, satisfies the following properties:

- For any event \mathcal{A} , its probability is never negative, i.e., $P(\mathcal{A}) \geq 0$;
- Probability of the entire sample space is 1, i.e., $P(\mathcal{S}) = 1$;
- For any countable sequence of events $\mathcal{A}_1, \mathcal{A}_2, \dots$ that are *mutually exclusive* ($\mathcal{A}_i \cap \mathcal{A}_j = \emptyset$ for all $i \neq j$), the probability that any happens is equal to the sum of their individual probabilities, i.e., $P(\bigcup_{i=1}^{\infty} \mathcal{A}_i) = \sum_{i=1}^{\infty} P(\mathcal{A}_i)$.

These are also the axioms of probability theory, proposed by Kolmogorov in 1933. Thanks to this axiom system, we can avoid any philosophical dispute on randomness; instead, we can reason rigorously with a mathematical language. For instance, by letting event \mathcal{A}_1 be the entire sample space and $\mathcal{A}_i = \emptyset$ for all $i > 1$, we can prove that $P(\emptyset) = 0$, i.e., the probability of an impossible event is 0.

Random Variables

In our random experiment of casting a die, we introduced the notion of a *random variable*. A random variable can be pretty much any quantity and is not deterministic. It could take one value among a set of possibilities in a random experiment. Consider a random variable X whose value is in the sample space $\mathcal{S} = \{1, 2, 3, 4, 5, 6\}$ of rolling a die. We can denote the event “seeing a 5” as $\{X = 5\}$ or $X = 5$, and its probability as $P(\{X = 5\})$ or $P(X = 5)$. By $P(X = a)$, we make a distinction between the random variable X and the values (e.g., a) that X can take. However, such pedantry results in a cumbersome notation. For a compact notation, on one hand, we can just denote $P(X)$ as the *distribution* over the random variable X : the distribution tells us the probability that X takes any value. On the other hand, we can simply write $P(a)$ to denote the probability that a random variable takes the value a . Since an event in probability theory is a set of outcomes from the sample space, we can specify a range of values for a random variable to take. For example, $P(1 \leq X \leq 3)$ denotes the probability of the event $\{1 \leq X \leq 3\}$, which means $\{X = 1, 2, \text{ or }, 3\}$. Equivalently, $P(1 \leq X \leq 3)$ represents the probability that the random variable X can take a value from $\{1, 2, 3\}$.

Note that there is a subtle difference between *discrete* random variables, like the sides of a die, and *continuous* ones, like the weight and the height of a person. There is little point in asking whether two people have exactly the same height. If we take precise enough measurements you will find that no two people on the planet have the exact same height. In fact, if we take a fine enough measurement, you will not have the same height when you wake up and when you go to sleep. So there is no purpose in asking about the probability that someone is 1.80139278291028719210196740527486202 meters tall. Given the world population of humans the probability is virtually 0. It makes more sense in this case to ask whether someone’s height falls into a given interval, say between 1.79 and 1.81 meters. In these cases we quantify the likelihood that we see a value as a *density*. The height of exactly 1.80 meters has no probability, but nonzero density. In the interval between any two different heights we have nonzero probability. In the rest of this section, we consider probability in discrete space. For probability over continuous random variables, you may refer to [Section 18.6](#).

2.6.2 Dealing with Multiple Random Variables

Very often, we will want to consider more than one random variable at a time. For instance, we may want to model the relationship between diseases and symptoms. Given a disease and a symptom, say “flu” and “cough”, either may or may not occur in a patient with some probability. While we hope that the probability of both would be close to zero, we may want to estimate these probabilities and their relationships to each other so that we may apply our inferences to effect better medical care.

As a more complicated example, images contain millions of pixels, thus millions of random variables. And in many cases images will come with a label, identifying objects in the image. We can also think of the label as a random variable. We can even think of all the metadata as random variables such as location, time, aperture, focal length, ISO, focus distance, and camera type. All of these are random variables that occur jointly. When we deal with multiple random variables, there are several quantities of interest.

Joint Probability

The first is called the *joint probability* $P(A = a, B = b)$. Given any values a and b , the joint probability lets us answer, what is the probability that $A = a$ and $B = b$ simultaneously? Note that for any values a and b , $P(A = a, B = b) \leq P(A = a)$. This has to be the case, since for $A = a$ and $B = b$ to happen, $A = a$ has to happen *and* $B = b$ also has to happen (and vice versa). Thus, $A = a$ and $B = b$ cannot be more likely than $A = a$ or $B = b$ individually.

Conditional Probability

This brings us to an interesting ratio: $0 \leq \frac{P(A=a, B=b)}{P(A=a)} \leq 1$. We call this ratio a *conditional probability* and denote it by $P(B = b | A = a)$: it is the probability of $B = b$, provided that $A = a$ has occurred.

Bayes' theorem

Using the definition of conditional probabilities, we can derive one of the most useful and celebrated equations in statistics: *Bayes' theorem*. It goes as follows. By construction, we have the *multiplication rule* that $P(A, B) = P(B | A)P(A)$. By symmetry, this also holds for $P(A, B) = P(A | B)P(B)$. Assume that $P(B) > 0$. Solving for one of the conditional variables we get

$$P(A | B) = \frac{P(B | A)P(A)}{P(B)}. \quad (2.6.1)$$

Note that here we use the more compact notation where $P(A, B)$ is a *joint distribution* and $P(A | B)$ is a *conditional distribution*. Such distributions can be evaluated for particular values $A = a, B = b$.

Marginalization

Bayes' theorem is very useful if we want to infer one thing from the other, say cause and effect, but we only know the properties in the reverse direction, as we will see later in this section. One important operation that we need, to make this work, is *marginalization*. It is the operation of determining $P(B)$ from $P(A, B)$. We can see that the probability of B amounts to accounting for all possible choices of A and aggregating the joint probabilities over all of them:

$$P(B) = \sum_A P(A, B), \quad (2.6.2)$$

which is also known as the *sum rule*. The probability or distribution as a result of marginalization is called a *marginal probability* or a *marginal distribution*.

Independence

Another useful property to check for is *dependence* vs. *independence*. Two random variables A and B being independent means that the occurrence of one event of A does not reveal any information about the occurrence of an event of B . In this case $P(B | A) = P(B)$. Statisticians typically express this as $A \perp B$. From Bayes' theorem, it follows immediately that also $P(A | B) = P(A)$. In all the other cases we call A and B dependent. For instance, two successive rolls of a die are independent. In contrast, the position of a light switch and the brightness in the room are not