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# Dive into Deep Learning

*Release 0.7*

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Just a few years ago, there were no legions of deep learning scientists developing intelligent products and services at major companies and startups. When the youngest of us (the authors) entered the field, machine learning didn't 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 forward-looking academic discipline with a narrow set of real-world applications. And those applications, e.g. speech recognition and computer vision, required so much domain knowledge that they were often regarded as separate areas entirely for which machine learning was one small component. Neural networks, the antecedents of the deep learning models that we focus on in this book, were regarded as outmoded tools.

In just the past five years, deep learning has taken the world by surprise, driving rapid progress in fields as diverse as computer vision, natural language processing, automatic speech recognition, reinforcement learning, and statistical modeling. With these advances in hand, we can now build cars that drive themselves (with increasing autonomy), smart reply systems that anticipate mundane replies, helping people dig out from mountains of email, and software agents that dominate the world's best humans at board games like Go, a feat once deemed to be decades away. Already, these tools are exerting a widening impact, changing the way movies are made, diseases are diagnosed, and playing a growing role in basic sciences – from astrophysics to biology. This book represents our attempt to make deep learning approachable, teaching you both the *concepts*, the *context*, and the *code*.

## 1.1 About This Book

### 1.1.1 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 on-boarding time needed 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 full potential of this technology to aid creative entrepreneurs has only been realized over the past ten years, owing to the development of powerful, well-documented frameworks.

Realizing 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 mathematics of a given modeling approach, (iii) the optimization algorithms for fitting the models to data, (iv) and the engineering required to train models efficiently, navigating the pitfalls of numerical computing and getting the most out of available hardware. Teaching 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.

We started this book project in July 2017 when we needed to explain MXNet’s (then new) Gluon interface to our users. At the time, there were no resources that were simultaneously (1) up to date, (2) covered the full breadth of modern machine learning with anything resembling of technical depth, and (3) interleaved the exposition one expects from an engaging textbook with the clean runnable code one seeks 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.) in the form of blog posts or on GitHub. 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 sporadic topics have been covered in blog posts, e.g. on the website [Distill<sup>1</sup>](#) or personal blogs, they only covered selected topics in deep learning, and often lacked associated code. On the other hand, while several textbooks have emerged, most notably [19], which offers an excellent survey of the concepts behind deep learning, these resources don’t 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 (1) be freely available for everyone, (2) offer sufficient technical depth to provide a starting point on the path to actually becoming an applied machine learning scientist, (3) include runnable code, showing readers *how* to solve problems in practice, (4) that allowed for rapid updates, both by us, and also by the community at large, and (5) be complemented by a [forum<sup>2</sup>](#) 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 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 17.6](#). We settled on Github to share the source and to allow for edits, 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.

### 1.1.2 Learning by Doing

Many textbooks teach a series of topics, each in exhaustive detail. For example, Chris Bishop’s excellent textbook [3], 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 beginners, this property limits its usefulness as an introductory text.

In this book, we’ll teach most concepts *just in time*. In other words, you’ll 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 notebook introduces both a reasonable number of new concepts and provides a single self-contained working example – using a real dataset. 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’s a big advantage to adhering to a policy of *1 working example, 1 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

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<sup>1</sup> <http://distill.pub>

<sup>2</sup> <http://discuss.mxnet.io>

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.

Throughout, we'll be working with the MXNet library, which has the rare property of being flexible enough for research while being fast enough for production. 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 Gluon's 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'll often present two versions of the example: one where we implement everything from scratch, relying only on NDArray and automatic differentiation, and another, more practical example, where we write succinct code using Gluon. Once we've taught you how some component works, we can just use the Gluon version in subsequent tutorials.

### 1.1.3 Content and Structure

The book can be roughly divided into three parts, which are presented by different colors in Fig. 1.1.1:

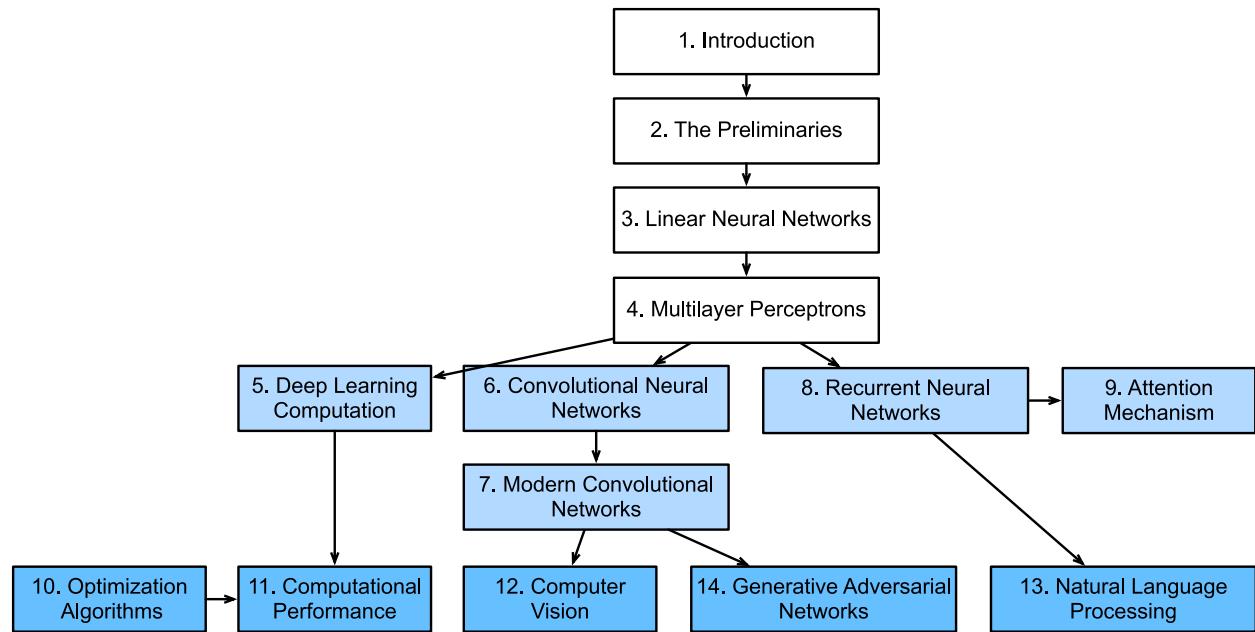


Fig. 1.1.1: Book structure

- The first part covers prerequisites and basics. The first chapter offers an introduction to deep learning in Section 3. In Section 4, we'll quickly bring you up to speed on the prerequisites required for hands-on deep learning, such as how to acquire and run the codes covered in the book. Section 5 and Section 6 cover the most basic concepts and techniques of deep learning, such as linear regression, multi-layer perceptrons and regularization.
- The next four chapters focus on modern deep learning techniques. Section 7 describes the various key components of deep learning calculations and lays the groundwork for the later implementation of more complex models. Next we explain in Section 8 and Section 9, powerful tools that form the backbone of most modern computer vision systems in recent years. Subsequently, we introduce Section 10 models that exploit temporal or sequential structure in data, and are commonly used for natural language processing and time series prediction. Section 11 introduces recent models exploring the attention mechanism. These sections will get you up to speed on the basic tools behind most modern deep learning.

- Part three discusses scalability, efficiency and applications. First, in [Section 12](#), we discuss several common optimization algorithms used to train deep learning models. The next chapter, [Section 13](#) examines several important factors that affect the computational performance of your deep learning code. [Section 14](#) and [Section 15](#) illustrate major applications of deep learning in computer vision and natural language processing, respectively. Finally, [Section 16](#) presents an emerging family of models called generative adversarial networks.

### 1.1.4 Code

Most sections of this book feature executable code. We recognize the importance of an interactive learning experience in deep learning. At present certain intuitions can only be developed through 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. Unfortunately, at present such elegant theories elude us. Despite our best attempts, our explanations of various techniques might be lacking, sometimes on account of our shortcomings, and equally often on account of the nascent state of the science of deep learning. We are hopeful that as the theory of deep learning progresses, future editions of this book will be able to provide insights in places the present edition cannot.

Most of the code in this book is based on Apache MXNet. MXNet is an open-source framework for deep learning and 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. However, we plan to keep the online version up-to-date. In case of such problems, please consult [Installation](#) (page 7) to update the code and runtime environment.

At times, to avoid unnecessary repetition, we encapsulate the frequently-imported and referred-to functions, classes, etc. in this book in the `d2l` package. For any block such as a function, a class, or multiple imports to be saved in the package, we will mark it with `# Save to the d2l package`. For example, these are the packages and modules used by the `d2l` package.

```
# Save to the d2l package
from IPython import display
import collections
import os
import sys
import numpy as np
import math
from matplotlib import pyplot as plt
from mxnet import nd, autograd, gluon, init, context, image
from mxnet.gluon import nn, rnn
import random
import re
import time
import tarfile
import zipfile
```

We give a detailed overview of these functions and classes in [Section 17.7](#).

### 1.1.5 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'll only assume that you come in with some basics, including (the very basics of) linear algebra, calculus, probability, and Python programming. Moreover, this book's appendix provides a refresher on most of the mathematics covered in this book. Most of the time, we will prioritize intuition and ideas over mathematical rigor. There are many terrific books which can lead the interested reader further. For instance Linear Analysis by Bela Bollobas [5] covers linear algebra and functional analysis in great depth. All of Statistics [63] is a terrific guide to statistics. And if you have not used Python before, you may want to peruse the [Python tutorial](#)<sup>3</sup>.

### 1.1.6 Forum

Associated with this book, we've launched a discussion forum, located at [discuss.mxnet.io](https://discuss.mxnet.io/)<sup>4</sup>. When you have questions on any section of the book, you can find the associated discussion page by scanning the QR code at the end of the section to participate in its discussions. The authors of this book and broader MXNet developer community frequently participate in forum discussions.

## 1.2 Acknowledgments

We are indebted to the hundreds of contributors for both the English and the Chinese drafts. They helped improve the content and offered valuable feedback. Specifically, we thank every contributor of this English draft for making it better for everyone. Their GitHub usernames or names are (in no particular order): alxnorden, avinashsingit, bowen0701, brettkoonce, Chaitanya Prakash Bapat, cryptonaut, Davide Fiocco, edgarroman, gkutiel, John Mitro, Liang Pu, Rahul Agarwal, mohamed-ali, mstewart141, Mike Müller, NRauschmayr, Prakhar Srivastav, sad-, sfermigier, Sheng Zha, sundeekteki, topecongiro, tpdi, vermicelli, Vishaal Kapoor, vishwesh5, YaYaB, Yuhong Chen, Evgeniy Smirnov, lgov, Simon Corston-Oliver, IgorDzreyev, trunghangx, pmuens, alukovenko, senorcinco, vfdev-5, dsweet, Mohammad Mahdi Rahimi, Abhishek Gupta, uwsd, DomKM, Lisa Oakley, bowen0701, arush15june, prasanth5reddy, brianhendee, mani2106, mtm, lkevinzc, caojilin, Lakshya, Fiete Lüer, Surbhi Vijayvargeeya, Muhyun Kim, dennismalmgren, adursun, Anirudh Dagar, liqingnz, Pedro Larroy, lgov, ati-ozgur, goldmermaid, Jun Wu, Matthias Blume, apeforest, geogunow, Josh Gardner, Maximilian Böther, rislam, Leonard Lausen, Abhinav Upadhyay, rongruosong, Steve Sedlmeyer, ruslo, Rafael Schlatter, liusy182, Giannis Pappas, ruslo, ati-ozgur, qbaza, dchoi77. Moreover, we thank Amazon Web Services, especially Swami Sivasubramanian, Raju Gulabani, Charlie Bell, and Andrew Jassy for their generous support in writing this book. Without the available time, resources, discussions with colleagues, and continuous encouragement this book would not have happened.

## 1.3 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.mxnet.io/>.

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<sup>3</sup> <http://learnpython.org/>

<sup>4</sup> <https://discuss.mxnet.io/>

- Apache MXNet is a powerful library for coding up deep learning models and running them in parallel across GPU cores.
- Gluon is a high level library that makes it easy to code up deep learning models using Apache MXNet.
- Conda is a Python package manager that ensures that all software dependencies are met.
- All notebooks are available for download on GitHub and the conda configurations needed to run this book’s code are expressed in the `environment.yml` file.
- If you plan to run this code on GPUs, don’t forget to install the necessary drivers and update your configuration.

## 1.4 Exercises

1. Register an account on the discussion forum of this book [discuss.mxnet.io](https://discuss.mxnet.io)<sup>5</sup>.
2. Install Python on your computer.
3. Follow the links at the bottom of the section to the forum, where you’ll be able to seek out help and discuss the book and find answers to your questions by engaging the authors and broader community.
4. Create an account on the forum and introduce yourself.

## 1.5 Scan the QR Code to Discuss<sup>6</sup>



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<sup>5</sup> <https://discuss.mxnet.io/>

<sup>6</sup> <https://discuss.mxnet.io/t/2311>

## INSTALLATION

To get you up and running with hands-on experiences, we'll need you to set up with a Python environment, Jupyter's interactive notebooks, the relevant libraries, and the code needed to *run the book*.

### 2.1 Obtaining Source Codes

The source code package containing all notebooks is available at <https://d2l.ai/d2l-en.zip>. Please download it and extract it into a folder. For example, on Linux/macOS, if you have both `wget` and `unzip` installed, you can do it through:

```
wget https://d2l.ai/d2l-en.zip
unzip d2l-en.zip -d d2l-en
```

### 2.2 Installing Running Environment

If you have both Python 3.5 or newer and pip installed, the easiest way to install the running environment through pip. Two packages are needed, `d2l` for all dependencies such as Jupyter and saved code blocks, and `mxnet` for deep learning framework we are using. First install `d2l` by

```
pip install d2l
```

If unfortunately something went wrong, please check

1. You are using `pip` for Python 3 instead of Python 2 by checking `pip --version`. If it's Python 2, then you may check if there is a `pip3` available.
2. You are using a recent `pip`, such as version 19. Otherwise you can upgrade it through `pip install --upgrade pip`
3. If you don't have permission to install package in system wide, you can install to your home directory by adding a `--user` flag. Such as `pip install d2l --user`

Before installing `mxnet`, please first check if you are able to access GPUs. If so, please go to [GPU Support](#) (page 8) for instructions to install a GPU-supported `mxnet`. Otherwise, we can install the CPU version, which is still good enough for the first few chapters.

```
pip install mxnet
```

Once both packages are installed, we now open the Jupyter notebook by

```
jupyter notebook
```

At this point open <http://localhost:8888> (which usually opens automatically) in the browser, then you can view and run the code in each section of the book.

## 2.3 Upgrade to a New Version

Both this book and MXNet are keeping improving. You may want to check a new version from time to time.

1. This URL <https://d2l.ai/d2l-en.zip> always points to the contents.
2. You can upgrade d2l by `pip install d2l -U` or even just install the latest version from Github by `pip install git+https://github.com/d2l-ai/d2l-en`.
3. MXNet can be upgraded by `pip install MXNet -U` as well.

## 2.4 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 CUDA<sup>7</sup>, you should install a GPU-enabled MXNet.

If you have installed the CPU-only version, then remove it first by

```
pip uninstall mxnet
```

Then you need to find the CUDA version you installed. You may check it through `nvcc --version` or `cat /usr/local/cuda/version.txt`. Assume you have installed CUDA 10.1, then you can install the according MXNet version by

```
pip install mxnet-cu101
```

You may change the last digits according to your CUDA version, e.g. `cu100` for CUDA 10.0 and `cu90` for CUDA 9.0. You can find all available MXNet versions by `pip search mxnet`.

## 2.5 Exercises

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

## 2.6 Scan the QR Code to Discuss<sup>8</sup>

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<sup>7</sup> <https://developer.nvidia.com/cuda-downloads>

<sup>8</sup> <https://discuss.mxnet.io/t/2315>





## INTRODUCTION

Until recently, nearly all of the computer programs that we interacted with every day were 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 would probably look something like this: (i) users would interact with the application through an interface running in a web browser or mobile application (ii) our application would rely on a commercial database engine to keep track of each user's state and maintain records of all historical transactions (ii) at the heart of our application, running in parallel across many servers, the *business logic* (you might say, the *brains*) would map out in methodical details the appropriate action to take in every conceivable circumstance.

To build the *brains* of our application, we'd 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're able to devise solutions that work 100% of the time, *you should not be using machine learning*.

Fortunately—for the growing community of ML scientists—many problems in automation don't bend so easily to human ingenuity. Imagine huddling around the whiteboard with the smartest minds you know, but this time you are tackling any 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 (ML) is the study of powerful techniques that can *learn behavior* from *experience*. As ML algorithm accumulates more experience, typically in the form of observational data or interactions with an environment, their 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's 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.

### 3.1 A Motivating Example

Before we could begin 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 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 smartphone can engage several machine learning models.

Imagine just writing a program to respond to a *wake word* like ‘Alexa’, ‘Okay, Google’ or ‘Siri’. Try coding it up in a room by yourself with nothing but a computer and a code editor. How would you write such a program from first principles? Think about it... the problem is hard. Every second, the microphone will collect roughly 44,000 samples. 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’re stuck, don’t worry. We don’t know how to write such a program from scratch either. That’s why we use ML.

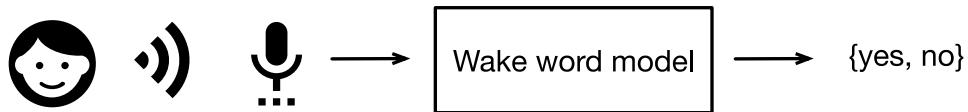


Fig. 3.1.1: Identify an awake word.

Here’s the trick. Often, even when we don’t 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 don’t know *how to program a computer* to recognize the word ‘Alexa’, you yourself *are able* to recognize the word ‘Alexa’. 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 ML approach, we do not 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 it generates a selection among {yes, no} as *output*—which, if all goes according to plan, will closely approximate whether (or not) the snippet contains the wake word.

If we choose the right family of models, then 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’ll probably need a model family capable, via another setting of the knobs, of firing **yes** on the word ‘Apricot’. We expect that the same model should apply to ‘Alexa’ recognition and ‘Apricot’ recognition because these are 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's not likely that our model will recognize 'Alexa', 'Apricot', or any other English word. In deep learning, the *learning* is the process by which we discover the right setting of the knobs coercing the desired behaviour from our model.

The training process usually looks like this:

1. Start off with a randomly initialized model that can't do anything useful.
2. Grab some of your labeled 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 until the model is awesome.

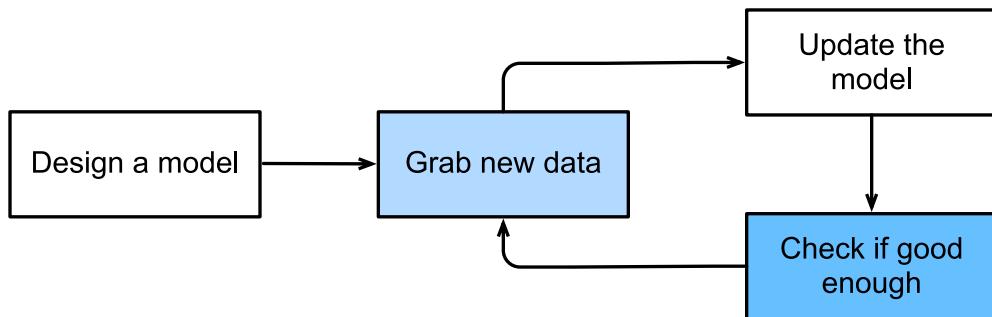


Fig. 3.1.2: A typical training process.

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*. We can "program" a cat detector by providing our machine learning system with many examples of cats and dogs, such as the images below:



This way the detector will eventually learn to emit a very large positive number if it's a cat, a very large negative number if it's a dog, and something closer to zero if it isn't sure, and this barely scratches the surface of what ML can do.

Deep learning is just one among many popular frameworks for solving machine learning problems. While thus far, we've only talked about machine learning broadly and not deep learning, there's a couple points worth sneaking in here: First, the problems that we've discussed thus far: learning from raw audio signal,

directly from the pixels in images, and mapping between sentences of arbitrary lengths and across languages are problems where deep learning excels and traditional ML tools faltered. Deep models are *deep* in precisely the sense that they learn many *layers* of computation. It turns out that these many-layered (or hierarchical) models are capable of addressing low-level perceptual data in a way that previous tools could not. In bygone days, the crucial part of applying ML to these problems consisted of coming up with manually engineered ways of transforming the data into some form amenable to *shallow* models. 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 feature engineering. Secondly, 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.

## 3.2 The Key Components: Data, Models, and Algorithms

In our *wake-word* example, we described a dataset consisting of audio snippets and binary labels 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* given known *inputs* (also called *features* or *covariates*), and examples of both is called *supervised learning*, and it's just one among many *kinds* of machine learning problems. In the next section, we'll take a deep dive into the different ML problems. First, we'd like to shed more light on some core components that will follow us around, no matter what kind of ML problem we take on:

1. The **data** that we can learn from
2. A **model** of how to transform the data
3. A **loss** function that quantifies the *badness* of our model
4. An **algorithm** to adjust the model's parameters to minimize the loss

### 3.2.1 Data

It might go without saying that you cannot do data science without data. We could lose hundreds of pages pondering the precise nature of data but for now we'll err on the practical side and focus on the key properties to be concerned with. Generally we are concerned with a collection of *examples* (also called *data points*, *samples*, or *instances*). In order to work with data usefully, we typically need to come up with a suitable numerical representation. Each *example* typically consists of a collection of numerical attributes called *features* or *covariates*.

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  $200 \times 200$  color photograph would consist of  $200 \times 200 \times 3 = 120000$  numerical values, corresponding to the brightness of the red, green, and blue channels corresponding to each spatial location. In a more 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, diagnoses, etc.

When every example is characterized by the same number of numerical values, we say that the data consists 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 means 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 can't expect images mined from the internet to all show up in the same size. While we might imagine cropping images to a standard size, text data resists fixed-length representations even more stubbornly. Consider the product reviews left on e-commerce sites like Amazon or

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 either don’t work without large data sets. Some others work in the low-data regime, but no better than traditional approaches.

Finally it’s not enough to have lots of data and to process it cleverly. We need the *right* data. If the data is 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 well captured by the cliché: *garbage in, garbage out*. Moreover, poor predictive performance isn’t the only potential consequence. In sensitive applications of machine learning, like predictive policing, resumé 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 doesn’t merely under-represent some groups, but reflects 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 being complicit, or even aware.

### 3.2.2 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 neural networks, we’ll discuss some more traditional methods.

### 3.2.3 Objective functions

Earlier, we introduced machine learning as “learning behavior 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  $f$  for which higher is better, and turn it into a new function  $f'$  that is qualitatively identical but for which lower is better by setting  $f' = -f$ . Because lower is better, these functions are sometimes called *loss functions* or *cost functions*.

When trying to predict numerical values, the most common objective function is squared error  $(y - \hat{y})^2$ . For classification, the most common objective is to minimize error rate, i.e., the fraction of instances on which our predictions disagree with the ground truth. Some objectives (like squared error) are easy to optimize.

Others (like error rate) are difficult to optimize directly, owing to non-differentiability or other complications. In these cases, it's common to optimize a surrogate objective.

Typically, the loss function is defined with respect to the model's parameters and depends upon the dataset. The best values of our model's parameters are learned by minimizing the loss incurred on a *training set* consisting of some number of *examples* collected for training. However, doing well on the training data doesn't guarantee that we will do well on (unseen) test data. So we'll typically want to split the available data into two partitions: the training data (for fitting model parameters) and the test data (which is held out for evaluation), reporting the following two quantities:

- **Training Error:** The error on that data on which the model was trained. You could think of this as being like a student's scores on practice exams used to prepare for some real exam. Even if the results are encouraging, that does not guarantee success on the final exam.
- **Test Error:** This is the error incurred on an unseen test set. This can deviate significantly from the training error. When a model 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.

### 3.2.4 Optimization algorithms

Once we've 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. The most popular optimization algorithms for neural networks follow an approach called gradient descent. In short, at each step, they check to see, for each parameter, which way the training set loss would move if you perturbed that parameter just a small amount. They then update the parameter in the direction that reduces the loss.

## 3.3 Kinds of Machine Learning

In the following sections, we will discuss a few types of machine learning in some more detail. We begin with a list of *objectives*, i.e. a list of things that machine learning can do. Note that the objectives are complemented with a set of techniques of *how* to accomplish them, i.e. training, types of data, etc. The list below is really only sufficient to whet the readers' appetite and to give us a common language when we talk about problems. We will introduce a larger number of such problems as we go along.

### 3.3.1 Supervised learning

Supervised learning addresses the task of predicting *targets* given input data. The targets, also commonly called *labels*, are generally denoted  $y$ . The input data points, also commonly called *examples* or *instances*, are typically denoted  $\mathbf{x}$ . The goal is to produce a model  $f_\theta$  that maps an input  $\mathbf{x}$  to a prediction  $f_\theta(\mathbf{x})$ .

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  $y$ . The input data  $\mathbf{x}$  might be vital signs such as heart rate, diastolic and systolic blood pressure, etc.

The supervision comes into play because for choosing the parameters  $\theta$ , we (the supervisors) provide the model with a collection of *labeled examples*  $(\mathbf{x}_i, y_i)$ , where each example  $\mathbf{x}_i$  is matched up against its correct label.

In probabilistic terms, we typically are interested in estimating the conditional probability  $P(y|\mathbf{x})$ . While it's just one among several approaches to machine learning, supervised learning accounts for the majority of machine learning in practice. Partly, that's because many important tasks can be described crisply as estimating the probability of some unknown given some available evidence:

- Predict cancer vs not cancer, given a CT 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 ‘predict targets from inputs’ supervised learning can take a great many forms and require a great many modeling decisions, depending on the type, size, and the number of inputs and outputs. For example, we use different models to process sequences (like strings of text or time series data) and for processing fixed-length vector representations. We'll visit many of these problems in depth throughout the first 9 parts of this book.

Put plainly, the learning process looks something like this. Grab a big pile of example inputs, selecting them randomly. Acquire the ground truth labels for each. Together, these inputs and corresponding labels (the desired outputs) comprise the training set. We feed the training dataset into a supervised learning algorithm. So here the *supervised learning algorithm* is a function that takes as input a dataset, and outputs another function, *the learned model*. Then, given a learned model, we can take a new previously unseen input, and predict the corresponding label.

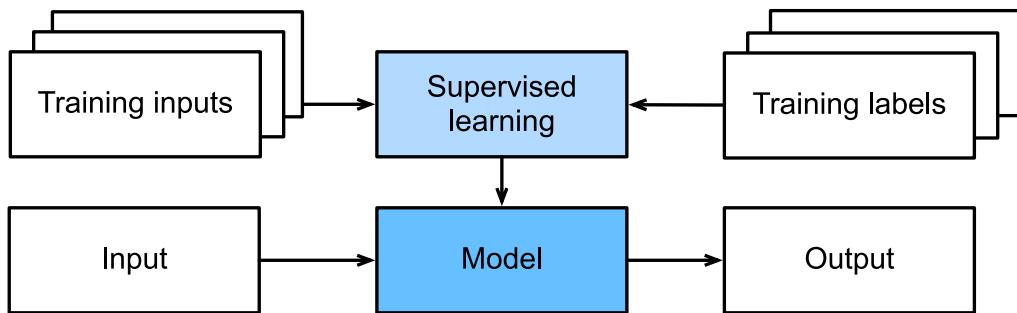


Fig. 3.3.1: Supervised learning.

## 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. Formally, we call one row in this dataset a *feature vector*, and the object (e.g. a house) it's associated with an *example*.

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: [100, 0, .5, 60]. However, if you live in Pittsburgh, it might look more like [3000, 4, 3, 10]. Feature vectors like this are essential for all the classic machine learning problems. We'll typically denote the feature vector for any one example  $\mathbf{x}_i$  and the set of feature vectors for all our examples  $X$ .

What makes a problem a *regression* is actually the outputs. Say that you're in the market for a new home, you might want to estimate the fair market value of a house, given some features like these. The target value, the price of sale, is a *real number*. We denote any individual target  $y_i$  (corresponding to example  $\mathbf{x}_i$ ) and the set of all targets  $\mathbf{y}$  (corresponding to all examples  $X$ ). When our targets take on arbitrary real values in some range, we call this a regression problem. The goal of our model is to produce predictions (guesses of the price, in our example) that closely approximate the actual target values. We denote these predictions  $\hat{y}_i$  and if the notation seems unfamiliar, then just ignore it for now. We'll unpack it more thoroughly in the subsequent chapters.

Lots of practical problems are well-described regression problems. Predicting the rating that a user will assign to a movie is a regression problem, and if you designed a great algorithm to accomplish this feat in 2009, you might have won the \$1 million Netflix prize<sup>9</sup>. 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.

- ‘How many hours will this surgery take?’ - *regression*
- ‘How many dogs are in this photo?’ - *regression*.

However, if you can easily pose your problem as ‘Is this a    ?’, then it’s likely, classification, a different fundamental problem type that we’ll cover next. Even if you’ve never worked with machine learning before, you’ve probably worked through a regression problem informally. Imagine, for example, that you had your drains repaired and that your contractor spent  $x_1 = 3$  hours removing gunk from your sewage pipes. Then she sent you a bill of  $y_1 = \$350$ . Now imagine that your friend hired the same contractor for  $x_2 = 2$  hours and that she received a bill of  $y_2 = \$250$ . 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’s some base charge and that the contractor then charges per hour. If these assumptions held true, then given these two data points, you could already identify the contractor’s pricing structure: \$100 per hour plus \$50 to show up at your house. If you followed that much then you already understand the high-level idea behind linear regression (and you just implicitly designed a linear model with bias).

In this case, we could produce the parameters that exactly matched the contractor’s prices. Sometimes that’s not possible, e.g., if some of the variance owes to some factors besides your two features. In these cases, we’ll try to learn models that minimize the distance between our predictions and the observed values. In most of our chapters, we’ll focus on one of two very common losses, the L1 loss<sup>10</sup> where

$$l(y, y') = \sum_i |y_i - y'_i| \quad (3.3.1)$$

and the least mean squares loss, aka L2 loss<sup>11</sup> where

$$l(y, y') = \sum_i (y_i - y'_i)^2. \quad (3.3.2)$$

As we will see later, the  $L_2$  loss corresponds to the assumption that our data was corrupted by Gaussian noise, whereas the  $L_1$  loss corresponds to an assumption of noise from a Laplace distribution.

## Classification

While regression models are great for addressing *how many?* questions, lots of problems don’t bend comfortably to this template. For example, a bank wants to add check scanning to their mobile app. This would involve the customer snapping a photo of a check with their smartphone’s camera and the machine learning model would need to be able to automatically understand text seen in the image. It would also need to understand hand-written text to be even more robust. This kind of system is referred to as optical character recognition (OCR), and the kind of problem it solves is called a classification. It’s treated with a distinct set of algorithms than those that are used for regression.

In classification, we want to look at a feature vector, like the pixel values in an image, and then predict which category (formally called *classes*), among some set of options, an example belongs. For hand-written digits, we might have 10 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  $X$  could consist of images of animals and our *labels*  $Y$  might be the classes {cat, dog}. While in regression,

<sup>9</sup> [https://en.wikipedia.org/wiki/Netflix\\_Prize](https://en.wikipedia.org/wiki/Netflix_Prize)

<sup>10</sup> <http://mxnet.incubator.apache.org/api/python/gluon/loss.html#mxnet.gluon.loss.L1Loss>

<sup>11</sup> <http://mxnet.incubator.apache.org/api/python/gluon/loss.html#mxnet.gluon.loss.L2Loss>

we sought a *regressor* to output a real value  $\hat{y}$ , in classification, we seek a *classifier*, whose output  $\hat{y}$  is the predicted class assignment.

For reasons that we'll get into as the book gets more technical, it's pretty hard to optimize a model that can only output a hard categorical assignment, e.g. either *cat* or *dog*. It's a lot easier instead to express the model in the language of probabilities. Given an example  $x$ , the model assigns a probability  $\hat{y}_k$  to each label  $k$ . Because these are probabilities, they need to be positive numbers and add up to 1. This means that we only need  $K - 1$  numbers to give the probabilities of  $K$  categories. This is easy to see for binary classification. If there's a 0.6 (60%) probability that an unfair coin comes up heads, then there's a 0.4 (40%) probability that it comes up tails. Returning to our animal classification example, a classifier might see an image and output the probability that the image is a cat  $\text{Pr}(y = \text{cat}|x) = 0.9$ . 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 is one notion of confidence. It's not the only notion of confidence and we'll discuss different notions of uncertainty 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, 3 ... 9, a, b, c, ...]. While we attacked regression problems by trying to minimize the L1 or L2 loss functions, the common loss function for classification problems is called cross-entropy. In MXNet Gluon, the corresponding loss function can be found [here](#)<sup>12</sup>.

Note that the most likely class is not necessarily the one that you're going to use for your decision. Assume that you find this beautiful mushroom in your backyard:



Fig. 3.3.2: Death cap - do not eat!

<sup>12</sup> <https://mxnet.incubator.apache.org/api/python/gluon/loss.html#mxnet.gluon.loss.SoftmaxCrossEntropyLoss>

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  $\Pr(y = \text{deathcap}|\text{image}) = 0.2$ . In other words, the classifier is 80% confident that our mushroom *is not* a death cap. Still, you'd have to be a fool to eat it. That's because the certain benefit of a delicious dinner isn't worth a 20% risk of dying from it. In other words, the effect of the *uncertain risk* by far outweighs the benefit. Let's look at this in math. Basically, we need to compute the expected risk that we incur, i.e. we need to multiply the probability of the outcome with the benefit (or harm) associated with it:

$$L(\text{action}|x) = \mathbf{E}_{y \sim p(y|x)} [\text{loss}(\text{action}, y)] \quad (3.3.3)$$

Hence, the loss  $L$  incurred by eating the mushroom is  $L(a = \text{eat}|x) = 0.2 * \infty + 0.8 * 0 = \infty$ , whereas the cost of discarding it is  $L(a = \text{discard}|x) = 0.2 * 0 + 0.8 * 1 = 0.8$ .

Our caution was justified: as any mycologist would tell us, the above mushroom 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 - we prefer to misclassify to a related class than to a distant class. Usually, this is referred to as *hierarchical classification*. One early example is due to Linnaeus<sup>13</sup>, who organized the animals in a hierarchy.

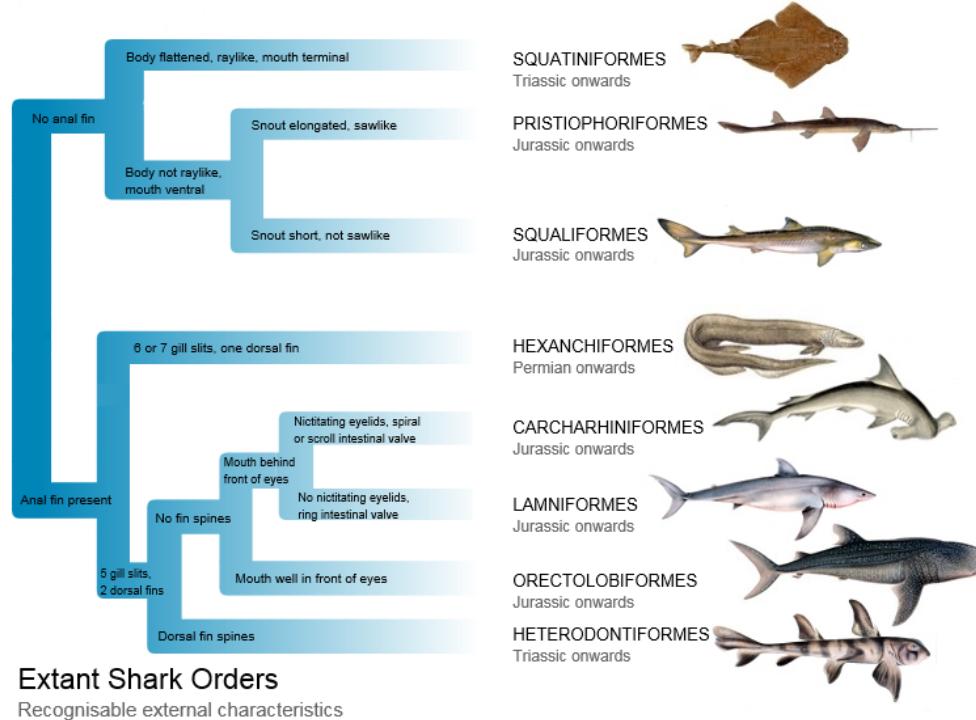


Fig. 3.3.3: Classify sharks

In the case of animal classification, it might not be so bad to mistake a poodle for a schnauzer, 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.

<sup>13</sup> [https://en.wikipedia.org/wiki/Carl\\_Linnaeus](https://en.wikipedia.org/wiki/Carl_Linnaeus)

## Tagging

Some classification problems don't 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.

As you can see, there's a cat in the picture, and a rooster, a dog, a donkey and a bird, 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 *and* a dog *and* a donkey *and* a rooster *and* a bird.

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 tech 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 28k 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 a competition<sup>14</sup> to do precisely this.

## Search and ranking

Sometimes we don't 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 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 should be displayed for the 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 nonetheless.

One possible solution to this problem is to score every element in the set of possible sets along with a corresponding relevance score and then to retrieve the top-rated elements. PageRank<sup>15</sup> is an early example of such a relevance score. One of the peculiarities is that it didn't depend on the actual query. Instead, it simply helped to order the results that contained the query terms. Nowadays search engines use machine learning and behavioral models to obtain query-dependent relevance scores. There are entire 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 SciFi fan and the results page for a connoisseur of Woody Allen comedies might differ significantly.

<sup>14</sup> <http://bioasq.org/>

<sup>15</sup> <https://en.wikipedia.org/wiki/PageRank>



Fig. 3.3.4: A cat, a roster, a dog and a donkey

Such problems occur, e.g. for movie, product or music recommendation. In some cases, customers will provide explicit details about how much they liked the product (e.g. Amazon product reviews). In some other cases, they might simply provide feedback if they are dissatisfied with the result (skipping titles on a playlist). Generally, such systems strive to estimate some score  $y_{ij}$ , such as an estimated rating or probability of purchase, given a user  $u_i$  and product  $p_j$ .

Given such a model, then for any given user, we could retrieve the set of objects with the largest scores  $y_{ij}$ , which are then used as a recommendation. Production systems are considerably more advanced and take detailed user activity and item characteristics into account when computing such scores. The following image is an example of deep learning books recommended by Amazon based on personalization algorithms tuned to the author's preferences.

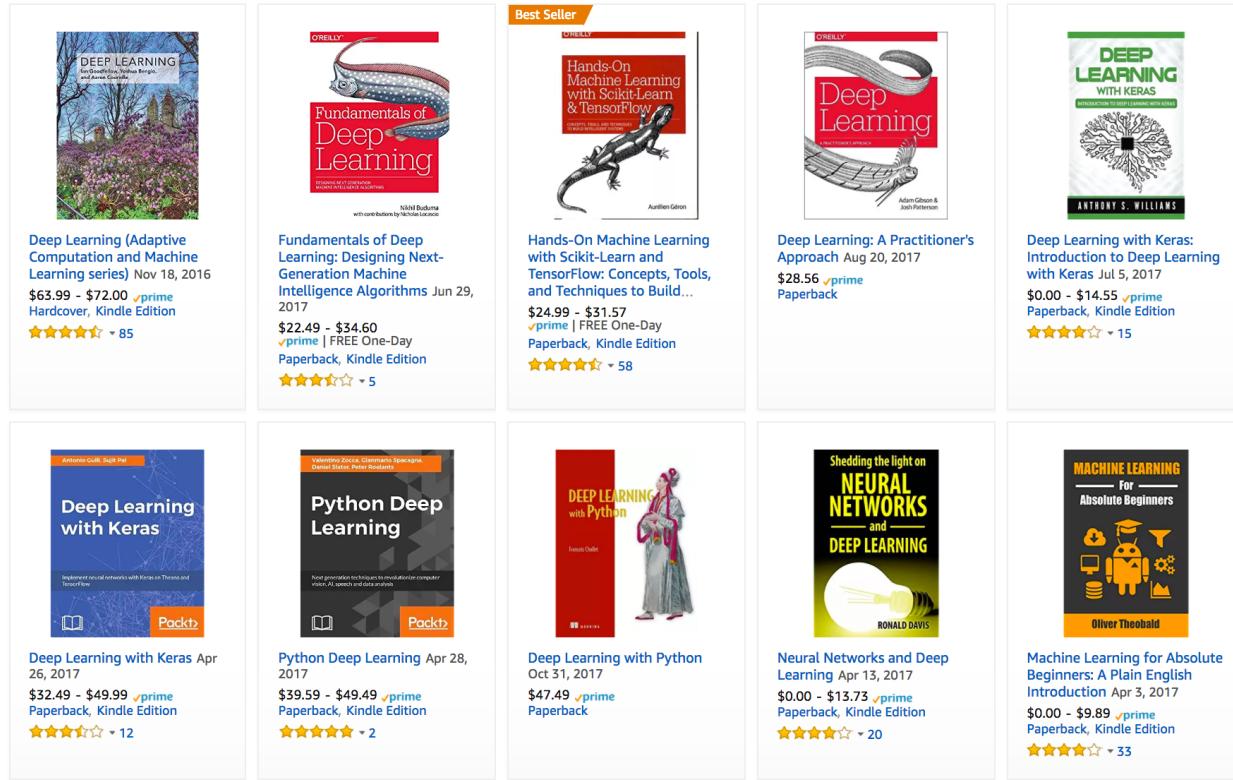


Fig. 3.3.5: Deep learning books recommended by Amazon.

## Sequence Learning

So far we've looked at problems where we have some fixed number of inputs and produce a fixed number of outputs. Before we considered predicting home 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's 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 wouldn't 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!). These latter problems are sometimes referred to as `seq2seq` problems. Language translation is a `seq2seq` problem. Transcribing text from spoken speech is also a `seq2seq` problem. While it is impossible to consider all types of sequence transformations, a number of 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.

Tom has dinner <b>in</b> Washington <b>with</b> Sally.	Ent	-	-	-	Ent	-	Ent
--	-----	---	---	---	-----	---	-----

### Automatic Speech Recognition

With speech recognition, the input sequence  $x$  is the sound of a speaker, and the output  $y$  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 correspond to a single spoken word. These are `seq2seq` problems where the output is much shorter than the input.

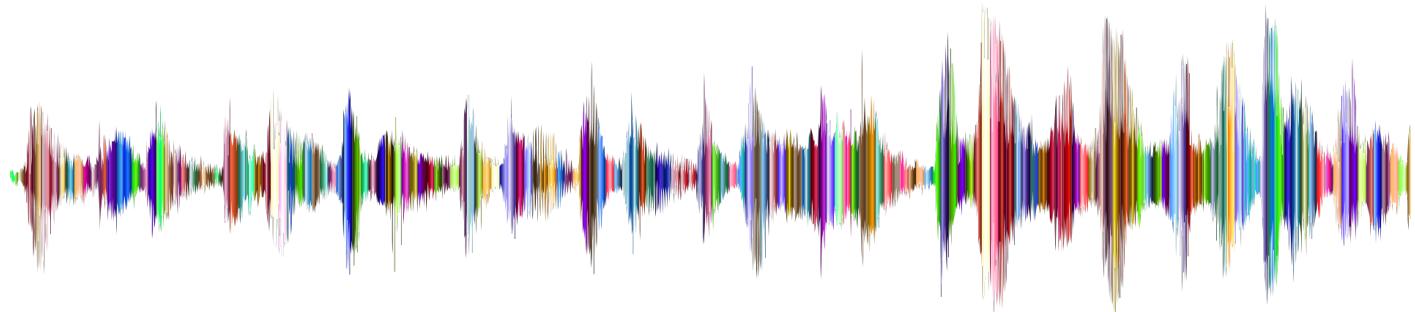


Fig. 3.3.6: -D-e-e-p- L-ea-r-ni-ng-

### Text to Speech

Text-to-Speech (TTS) is the inverse of speech recognition. In other words, the input  $x$  is text and the output  $y$  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 isn't 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 points are assumed to be the same. Consider the following illustrative example of the obnoxious 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?

A number of related problems exist. For instance, determining the order in which a user reads a webpage is a two-dimensional layout analysis problem. Likewise, for dialogue problems, we need to take world-knowledge and prior state into account. This is an active area of research.

### 3.3.2 Unsupervised learning

All the examples so far were related to *Supervised Learning*, i.e. situations where we feed the model a bunch of examples and a bunch of *corresponding target values*. You could think of supervised learning as having an extremely specialized job and an extremely anal 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's 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'd 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 a number of unsupervised learning techniques in later chapters. To whet your appetite for now, we describe a few of the 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, mountain peaks, etc.? Likewise, given a collection of users' browsing activity, 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** problems. If the dependence is linear, it is called **principal component analysis**.
- Is there a representation of (arbitrarily structured) objects in Euclidean space (i.e. the space of vectors in  $\mathbb{R}^n$ ) such that symbolic properties can be well matched? This is called **representation learning** and it is 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, salaries, etc., can we discover how they are related simply based on empirical data? The field of **directed graphical models** and **causality** deals with this.

- An important and exciting recent development is **generative adversarial networks**. They are basically a procedural way of synthesizing data. The underlying statistical mechanisms are tests to check whether real and fake data are the same. We will devote a few notebooks to them.

### 3.3.3 Interacting with an Environment

So far, we haven't discussed where data actually comes from, or what actually *happens* when a machine learning model generates an output. That's 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 up front, then do our pattern recognition without ever interacting with the environment again. Because all of the learning takes place after the algorithm is disconnected from the environment, this is called *offline learning*. For supervised learning, the process looks like this:

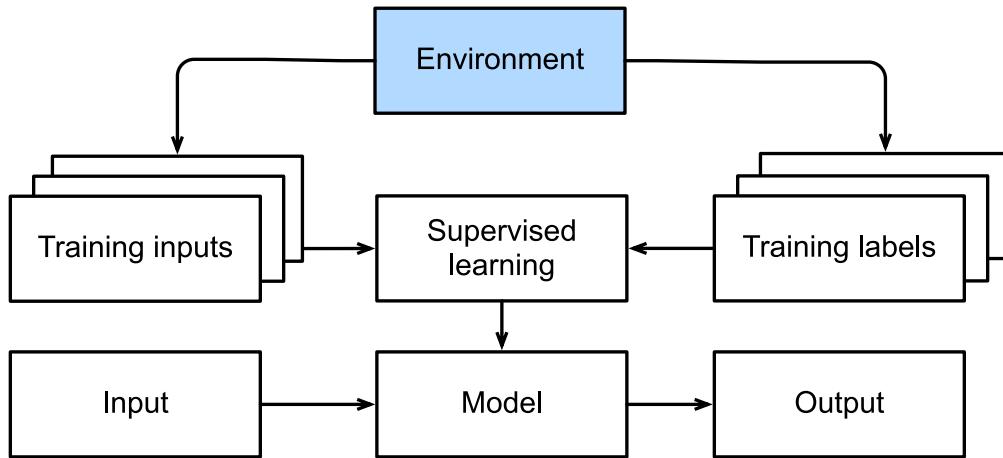


Fig. 3.3.7: Collect data for supervised learning from an environment.

This simplicity of offline learning has its charms. The upside is we can worry about pattern recognition in isolation without these other problems to deal with, 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 of taking actions in the world. We want to think about intelligent *agents*, not just predictive *models*. That means 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. Does the environment:

- remember what we did previously?
- want to help us, e.g. a user reading text into a speech recognizer?
- want to beat us, i.e. an adversarial setting like spam filtering (against spammers) or playing a game (vs an opponent)?
- not care (as in most cases)?
- have shifting dynamics (steady vs. shifting over time)?

This last question raises the problem of *covariate shift*, (when training and test data are different). It's a problem that most of us have experienced when taking exams written by a lecturer, while the homeworks were composed by his TAs. We'll briefly describe reinforcement learning and adversarial learning, two settings that explicitly consider interaction with an environment.

### 3.3.4 Reinforcement learning

If you're interested in using machine learning to develop an agent that interacts with an environment and takes actions, then you're probably going to wind up focusing on *reinforcement learning* (RL). This might include applications to robotics, to dialogue systems, and even to developing AI for video games. *Deep reinforcement learning* (DRL), which applies deep neural networks to RL problems, has surged in popularity. The breakthrough *deep Q-network* that beat humans at Atari games using only the visual input<sup>16</sup>, and the *AlphaGo* program that dethroned the world champion at the board game Go<sup>17</sup> 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  $t$ , the agent receives some observation  $o_t$  from the environment, and must choose an action  $a_t$  which is then transmitted back to the environment. Finally, the agent receives a reward  $r_t$  from the environment. The agent then receives a subsequent observation, and chooses a subsequent action, and so on. The behavior of an RL 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.

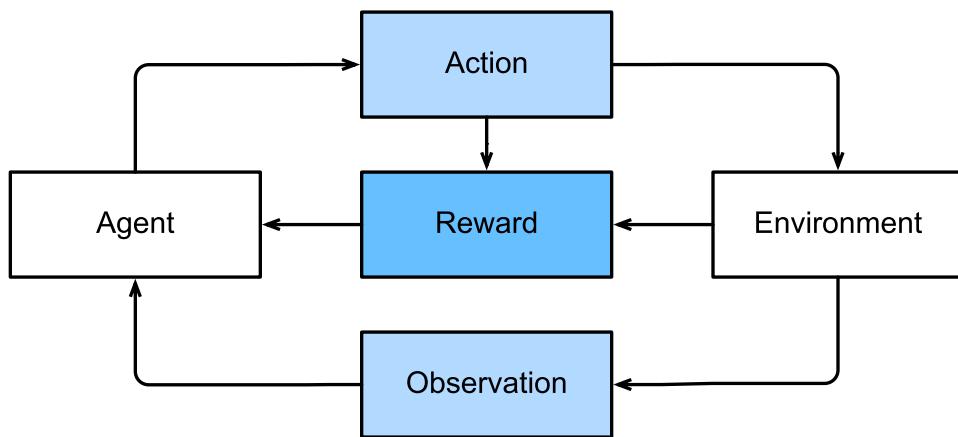


Fig. 3.3.8: The interaction between reinforcement learning and an environment.

It's hard to overstate the generality of the RL framework. For example, we can cast any supervised learning problem as an RL problem. Say we had a classification problem. We could create an RL 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 problem.

That being said, RL 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 RL, we don't 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*. 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

<sup>16</sup> <https://www.wired.com/2015/02/google-ai-plays-atari-like-pros/>

<sup>17</sup> <https://www.wired.com/2017/05/googles-alphago-trounces-humans-also-gives-boost/>

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.

### MDPs, bandits, and friends

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 RL problem a *Markov Decision Process* (MDP). 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*.

## 3.4 Roots

Although deep learning is a recent invention, humans have held the desire to analyze data and to predict future outcomes for centuries. In fact, much of natural science has its roots in this. For instance, the Bernoulli distribution is named after Jacob Bernoulli (1655-1705)<sup>18</sup>, and the Gaussian distribution was discovered by Carl Friedrich Gauss (1777-1855)<sup>19</sup>. He invented for instance the least mean squares algorithm, which is still used today for a range of problems from insurance calculations to medical diagnostics. These tools gave rise to an experimental approach in 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)<sup>20</sup> illustrates averaging the length of 16 adult men's feet to obtain the average foot length.

Figure 1.1 illustrates how this estimator works. 16 adult men were asked to line up in a row, when leaving 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.

Statistics really took off with the collection and availability of data. One of its titans, Ronald Fisher (1890-1962)<sup>21</sup>, contributed significantly to its theory and also its applications in genetics. Many of his algorithms (such as Linear Discriminant Analysis) and formulae (such as the Fisher Information Matrix) are still in frequent use today (even the Iris dataset that he released in 1936 is still used sometimes to illustrate machine learning algorithms).

A second influence for machine learning came from Information Theory (Claude Shannon, 1916-2001)<sup>22</sup> and the Theory of computation via Alan Turing (1912-1954)<sup>23</sup>. Turing posed the question "can machines

<sup>18</sup> [https://en.wikipedia.org/wiki/Jacob\\_Bernoulli](https://en.wikipedia.org/wiki/Jacob_Bernoulli)

<sup>19</sup> [https://en.wikipedia.org/wiki/Carl\\_Friedrich\\_Gauss](https://en.wikipedia.org/wiki/Carl_Friedrich_Gauss)

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

<sup>21</sup> [https://en.wikipedia.org/wiki/Ronald\\_Fisher](https://en.wikipedia.org/wiki/Ronald_Fisher)

<sup>22</sup> [https://en.wikipedia.org/wiki/Claude\\_Shannon](https://en.wikipedia.org/wiki/Claude_Shannon)

<sup>23</sup> [https://en.wikipedia.org/wiki/Alan\\_Turing](https://en.wikipedia.org/wiki/Alan_Turing)



Fig. 3.4.1: Estimating the length of a foot

think?” in his famous paper Computing machinery and intelligence<sup>24</sup> (Mind, October 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 being through textual interactions. To this day, the development of intelligent machines is changing rapidly and continuously.

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 these insights. One of the oldest algorithms to accomplish this was formulated by Donald Hebb (1904-1985)<sup>25</sup>.

In his groundbreaking book The Organization of Behavior<sup>26</sup> (John Wiley & Sons, 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 weights in a neural network.

Biological inspiration is what gave Neural Networks its 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 became more loose 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 (aka 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

<sup>24</sup> [https://en.wikipedia.org/wiki/Computing\\_Machinery\\_and\\_Intelligence](https://en.wikipedia.org/wiki/Computing_Machinery_and_Intelligence)

<sup>25</sup> [https://en.wikipedia.org/wiki/Donald\\_O.\\_Hebb](https://en.wikipedia.org/wiki/Donald_O._Hebb)

<sup>26</sup> [http://s-f-walker.org.uk/pubsebooks/pdfs/The\\_Organization\\_of\\_Behavior-Donald\\_O.\\_Hebb.pdf](http://s-f-walker.org.uk/pubsebooks/pdfs/The_Organization_of_Behavior-Donald_O._Hebb.pdf)

due to a number of reasons. Training a network is computationally very expensive. While RAM was plentiful at the end of the past century, computational power was scarce. Secondly, datasets were relatively small. In fact, Fisher’s ‘Iris dataset’ from 1932 was a popular tool for testing the efficacy of algorithms. MNIST with its 60,000 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.

## 3.5 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 3.5.1](#).

Table 3.5.1: Dataset versus 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 quite evident that RAM 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 needed to become more memory efficient (this is typically achieved by adding nonlinearities) while simultaneously being able to spend more time on optimizing these parameters, due to an increased compute budget. Consequently the sweet spot in machine learning and statistics moved from (generalized) linear models and kernel methods to deep networks. This is also one of the reasons why many of the mainstays of deep learning, such as Multilayer Perceptrons ([\[45\]](#)), Convolutional Neural Networks ([\[34\]](#)), Long Short Term Memory ([\[24\]](#)), Q-Learning ([\[64\]](#)), were essentially ‘rediscovered’ in the past decade, after laying 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 [\[55\]](#) allowed for training of relatively large networks without the danger of overfitting, i.e. without the danger of merely memorizing large parts of the training data. This was achieved by applying noise injection [\[2\]](#) throughout the 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. [\[1\]](#) found an elegant solution by using what can only be viewed as a learnable pointer structure. That is, rather than having to remember an entire sentence, 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 sentences, since the model no longer needed to remember the entire sentence before beginning to generate sentences.

- Multi-stage designs, e.g. via the Memory Networks [56] and the Neural Programmer-Interpreter [50] allowed statistical modelers to describe iterative approaches to reasoning. These tools allow for an internal state of the deep 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 [20]. 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 GANs 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 [71] and of fake celebrity faces [29] are both testimony to this progress.
- 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 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 32k images. Recent work, first by Li [35], and subsequently by [69] and [28] pushed the size up to 64k observations, reducing training time for ResNet50 on ImageNet 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. [53] 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 Caffe<sup>27</sup>, Torch<sup>28</sup>, and Theano<sup>29</sup>. Many seminal papers were written using these tools. By now they have been superseded by TensorFlow<sup>30</sup>, often used via its high level API Keras<sup>31</sup>, CNTK<sup>32</sup>, Caffe 2<sup>33</sup>, and Apache MxNet<sup>34</sup>. The third generation of tools, namely imperative tools for deep learning, was arguably spearheaded by Chainer<sup>35</sup>, which used a syntax similar to Python NumPy to describe models. This idea was adopted by PyTorch<sup>36</sup> and the Gluon API<sup>37</sup> of MXNet. It is the latter that this course uses to teach Deep Learning.

The division of labor between systems researchers building better tools for training and statistical modelers building better 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 PhD students at Carnegie Mellon University in 2014. By now, this task can be accomplished with less than 10 lines of code,

<sup>27</sup> <https://github.com/BVLC/caffe>

<sup>28</sup> <https://github.com/torch>

<sup>29</sup> <https://github.com/Theano/Theano>

<sup>30</sup> <https://github.com/tensorflow/tensorflow>

<sup>31</sup> <https://github.com/keras-team/keras>

<sup>32</sup> <https://github.com/Microsoft/CNTK>

<sup>33</sup> <https://github.com/caffe2/caffe2>

<sup>34</sup> <https://github.com/apache/incubator-mxnet>

<sup>35</sup> <https://github.com/chainer/chainer>

<sup>36</sup> <https://github.com/pytorch/pytorch>

<sup>37</sup> <https://github.com/apache/incubator-mxnet>

putting it firmly into the grasp of programmers.

## 3.6 Success Stories

Artificial Intelligence has a long history of delivering results that would be difficult to accomplish otherwise. For instance, mail is sorted using optical character recognition. These systems have been deployed since the 90s (this is, after all, the source of the famous MNIST and USPS sets 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, MasterCard. Computer programs for chess have been competitive for decades. Machine learning feeds search, recommendation, personalization and ranking on the internet. In other words, artificial intelligence and machine learning are 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.

- Intelligent assistants, such as Apple’s Siri, Amazon’s Alexa, or 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 [68] for certain applications.
- 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 [38] achieved a top-5 error rate of 28%. By 2017, [25] reduced this error rate to 2.25%. Similarly stunning results have been achieved for identifying birds, or diagnosing skin cancer.
- Games used to be a bastion of human intelligence. Starting from TDGammon [23], a program for playing Backgammon using temporal difference (TD) 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 Gary Kasparov, Campbell et al. [8], using massive parallelism, special purpose hardware and efficient search through the game tree. Go is more difficult still, due to its huge state space. AlphaGo reached human parity in 2015, [53] using Deep Learning combined with Monte Carlo tree sampling. The challenge in Poker was that the state space is large and it is not fully observed (we don’t know the opponents’ cards). Libratus exceeded human performance in Poker using efficiently structured strategies [7]. 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 Momenta, Tesla, NVIDIA, MobilEye 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 what is considered intelligent and where machine learning has led to impressive progress in a field. 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. ML 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 cars safely, decisions about whether to grant bail use statistical data as input. More frivolously, we can ask Alexa to switch on the coffee machine and she will happily oblige, provided that the appliance is internet enabled.

Fortunately we are far from a sentient AI system that is ready to enslave its human creators (or burn their coffee). Firstly, 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 general Artificial 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 realistic 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 will have profound consequences on large swaths of society (truck drivers and shop assistants are some of the most common jobs in many states). Furthermore, statistical models, when applied without care can lead to racial, gender or age bias. It is important to ensure that these algorithms are used with great care. This is a much bigger concern than to worry about a potentially malevolent superintelligence intent on destroying humanity.

## 3.7 Summary

- Machine learning studies how computer systems can use data to improve performance. It combines ideas from statistics, data mining, artificial intelligence and optimization. Often it is used as a means of implementing artificially intelligent solutions.
- As a class of machine learning, representational learning focuses on how to automatically find the appropriate way to represent data. This is often accomplished by a progression of learned transformations.
- Much of the recent progress 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 good performance. The availability of efficient deep learning frameworks has made design and implementation of this significantly easier.

## 3.8 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 Artificial Intelligence 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? Physics? Engineering? Econometrics?

### 3.9 Scan the QR Code to Discuss<sup>38</sup>



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<sup>38</sup> <https://discuss.mxnet.io/t/2310>

## THE PRELIMINARIES: A CRASHCOURSE

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 and manipulating data with Apache MXNet. 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 won't go too far into the weeds but rather focus on the basic of matrix operations and their implementation in Apache MXNet. 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. Fortunately, Apache MXNet's autograd package covers this 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 and statistics. To conclude the chapter, we will present your first basic classifier, *Naive Bayes*.

### 4.1 Data Manipulation

It is impossible to get anything done if we cannot manipulate data. Generally, there are two important things we need to do with data: (i) acquire it and (ii) process it once it is inside the computer. There is no point in acquiring data if we do not even know how to store it, so let's get our hands dirty first by playing with synthetic data. We will start by introducing the NDArray, MXNet's primary tool for storing and transforming data. If you have worked with NumPy before, you will notice that NDArrays are, by design, similar to NumPy's multi-dimensional array. However, they confer a few key advantages. First, NDArrays support asynchronous computation on CPU, GPU, and distributed cloud architectures. Second, they provide support for automatic differentiation. These properties make NDArray indispensable for deep learning.

#### 4.1.1 Getting Started

Throughout this chapter, we are aiming to get you up and running with the basic functionality. Do not worry if you do not understand all of the basic math, like element-wise operations or normal distributions. In the next two chapters we will take another pass at the same material, teaching the material in the context of practical examples. On the other hand, if you want to go deeper into the mathematical content, see Section 17.2.

We begin by importing MXNet and the `ndarray` module from MXNet. Here, `nd` is short for `ndarray`.

```
from mxnet import nd
```

NDArrays represent (possibly multi-dimensional) arrays of numerical values. NDArrays with one axis correspond (in math-speak) to *vectors*. NDArrays with two axes correspond to *matrices*. For arrays with more than two axes, mathematicians do not have special names—they simply call them *tensors*.

The simplest object we can create is a vector. To start, we can use `arange` to create a row vector with 12 consecutive integers.

```
x = nd.arange(12)
x
```

```
[ 0.  1.  2.  3.  4.  5.  6.  7.  8.  9. 10. 11.]
<NDArray 12 @cpu(0)>
```

When we print `x`, we can observe the property `<NDArray 12 @cpu(0)>` listed, which indicates that `x` is a one-dimensional array of length 12 and that it resides in CPU main memory. The 0 in `@cpu(0)` has no special meaning and does not represent a specific core.

We can get the NDArray instance shape through the `shape` property.

```
x.shape
```

```
(12,)
```

We can also get the total number of elements in the NDArray instance through the `size` property. This is the product of the elements of the shape. Since we are dealing with a vector here, both are identical.

```
x.size
```

```
12
```

We use the `reshape` function to change the shape of one (possibly multi-dimensional) array, to another that contains the same number of elements. For example, we can transform the shape of our line vector `x` to `(3, 4)`, which contains the same values but interprets them as a matrix containing 3 rows and 4 columns. Note that although the shape has changed, the elements in `x` have not. Moreover, the `size` remains the same.

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

```
[[ 0.  1.  2.  3.]
 [ 4.  5.  6.  7.]
 [ 8.  9. 10. 11.]]
<NDArray 3x4 @cpu(0)>
```

Reshaping by manually specifying each of the dimensions can get annoying. Once we know one of the dimensions, why should we have to perform the division ourselves to determine the other? For example, above, to get a matrix with 3 rows, we had to specify that it should have 4 columns (to account for the 12 elements). Fortunately, NDArray can automatically work out one dimension given the other. We can invoke this capability by placing `-1` for the dimension that we would like NDArray to automatically infer. In our case, instead of `x.reshape((3, 4))`, we could have equivalently used `x.reshape((-1, 4))` or `x.reshape((3, -1))`.

```
nd.empty((3, 4))
```

```
[[ -3.8194709e-21 4.5640291e-41 2.3407984e-28 3.0845382e-41]
 [ 0.0000000e+00 0.0000000e+00 0.0000000e+00 0.0000000e+00]
 [ 0.0000000e+00 0.0000000e+00 0.0000000e+00 0.0000000e+00]]
<NDArray 3x4 @cpu(0)>
```

The `empty` method just grabs some memory and hands us back a matrix without setting the values of any of its entries. This is very efficient but it means that the entries might take any arbitrary values, including very big ones! Typically, we'll want our matrices initialized either with ones, zeros, some known constant or numbers randomly sampled from a known distribution.

Perhaps most often, we want an array of all zeros. To create an NDArray representing a tensor with all elements set to 0 and a shape of (2, 3, 4) we can invoke:

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

```
[[[0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]]

 [[0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]]]
<NDArray 2x3x4 @cpu(0)>
```

We can create tensors with each element set to 1 works via

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

```
[[[1. 1. 1. 1.]
 [1. 1. 1. 1.]
 [1. 1. 1. 1.]]

 [[1. 1. 1. 1.]
 [1. 1. 1. 1.]
 [1. 1. 1. 1.]]]
<NDArray 2x3x4 @cpu(0)>
```

We can also specify the value of each element in the desired NDArray by supplying a Python list containing the numerical values.

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

```
[[2. 1. 4. 3.]
 [1. 2. 3. 4.]
 [4. 3. 2. 1.]]
<NDArray 3x4 @cpu(0)>
```

In some cases, we will want to randomly sample the values of each element in the NDArray according to some known probability distribution. This is especially common when we intend to use the array as a parameter in a neural network. The following snippet creates an NDArray with a shape of (3,4). Each of its elements is randomly sampled in a normal distribution with zero mean and unit variance.

```
nd.random.normal(0, 1, shape=(3, 4))
```

```
[[ 2.2122064   0.7740038   1.0434405   1.1839255 ]
 [ 1.8917114  -1.2347414  -1.771029   -0.45138445]
 [ 0.57938355 -1.856082   -1.9768796  -0.20801921]]
<NDArray 3x4 @cpu(0)>
```

## 4.1.2 Operations

Oftentimes, we want to apply functions to arrays. Some of the simplest and most useful functions are the element-wise functions. These operate by performing a single scalar operation on the corresponding elements of two arrays. We can create an element-wise function from any function that maps from the scalars to the scalars. In math notations we would denote such a function as  $f : \mathbb{R} \rightarrow \mathbb{R}$ . Given any two vectors  $\mathbf{u}$  and  $\mathbf{v}$  of the same shape, and the function  $f$ , we can produce a vector  $\mathbf{c} = F(\mathbf{u}, \mathbf{v})$  by setting  $c_i \leftarrow f(u_i, v_i)$  for all  $i$ . Here, we produced the vector-valued  $F : \mathbb{R}^d \rightarrow \mathbb{R}^d$  by *lifting* the scalar function to an element-wise vector operation. In MXNet, the common standard arithmetic operators (+,-,/,\*,\*\*) have all been *lifted* to element-wise operations for identically-shaped tensors of arbitrary shape. We can call element-wise operations on any two tensors of the same shape, including matrices.

```
x = nd.array([1, 2, 4, 8])
y = nd.ones_like(x) * 2
print('x =', x)
print('x + y', x + y)
print('x - y', x - y)
print('x * y', x * y)
print('x / y', x / y)
```

```
x =
[1. 2. 4. 8.]
<NDArray 4 @cpu(0)>
x + y
[ 3.  4.  6. 10.]
<NDArray 4 @cpu(0)>
x - y
[-1.  0.  2.  6.]
<NDArray 4 @cpu(0)>
x * y
[ 2.  4.  8. 16.]
<NDArray 4 @cpu(0)>
x / y
[0.5 1.  2.  4. ]
<NDArray 4 @cpu(0)>
```

Many more operations can be applied element-wise, such as exponentiation:

```
x.exp()
```

```
[2.7182817e+00 7.3890562e+00 5.4598148e+01 2.9809580e+03]
<NDArray 4 @cpu(0)>
```

In addition to computations by element, we can also perform matrix operations, like matrix multiplication using the dot function. Next, we will perform matrix multiplication of  $\mathbf{x}$  and the transpose of  $\mathbf{y}$ . We define

`x` as a matrix of 3 rows and 4 columns, and `y` is transposed into a matrix of 4 rows and 3 columns. The two matrices are multiplied to obtain a matrix of 3 rows and 3 columns (if you are confused about what this means, do not worry - we will explain matrix operations in much more detail in Section 4.2).

```
x = nd.arange(12).reshape((3,4))
y = nd.array([[2, 1, 4, 3], [1, 2, 3, 4], [4, 3, 2, 1]])
nd.dot(x, y.T)
```

```
[[ 18.  20.  10.]
 [ 58.  60.  50.]
 [ 98. 100.  90.]]
<NDArray 3x3 @cpu(0)>
```

We can also merge multiple NDArrays. For that, we need to tell the system along which dimension to merge. The example below merges two matrices along dimension 0 (along rows) and dimension 1 (along columns) respectively.

```
nd.concat(x, y, dim=0)
nd.concat(x, y, dim=1)
```

```
[[ 0.  1.  2.  3.  2.  1.  4.  3.]
 [ 4.  5.  6.  7.  1.  2.  3.  4.]
 [ 8.  9. 10. 11.  4.  3.  2.  1.]]
<NDArray 3x8 @cpu(0)>
```

Sometimes, we may want to construct binary NDArrays via logical statements. Take `x == y` as an example. If `x` and `y` are equal for some entry, the new ndarray has a value of 1 at the same position; otherwise it is 0.

```
x == y
```

```
[[0.  1.  0.  1.]
 [0.  0.  0.  0.]
 [0.  0.  0.  0.]]
<NDArray 3x4 @cpu(0)>
```

Summing all the elements in the ndarray yields an ndarray with only one element.

```
x.sum()
```

```
[66.]
<NDArray 1 @cpu(0)>
```

We can transform the result into a scalar in Python using the `asscalar` function. In the following example, the  $\ell_2$  norm of `x` yields a single element ndarray. The final result is transformed into a scalar.

```
x.norm().asscalar()
```

```
22.494442
```

For stylistic convenience, we can write `y.exp()`, `x.sum()`, `x.norm()`, etc. also as `nd.exp(y)`, `nd.sum(x)`, `nd.norm(x)`.

### 4.1.3 Broadcast Mechanism

In the above section, we saw how to perform operations on two NDArrays of the same shape. When their shapes differ, a broadcasting mechanism may be triggered analogous to NumPy: first, copy the elements appropriately so that the two NDArrays have the same shape, and then carry out operations by element.

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

```
(
[[0.]
 [1.]
 [2.]]
<NDArray 3x1 @cpu(0)>,
 [[0. 1.]]
<NDArray 1x2 @cpu(0)>)
```

Since `a` and `b` are (3x1) and (1x2) matrices respectively, their shapes do not match up if we want to add them. NDArray addresses this by ‘broadcasting’ the entries of both matrices into a larger (3x2) matrix as follows: for matrix `a` it replicates the columns, for matrix `b` it replicates the rows before adding up both element-wise.

```
a + b
```

```
[[0. 1.]
 [1. 2.]
 [2. 3.]]
<NDArray 3x2 @cpu(0)>
```

### 4.1.4 Indexing and Slicing

Just like in any other Python array, elements in an NDArray can be accessed by its index. In good Python tradition the first element has index 0 and ranges are specified to include the first but not the last element. By this logic `1:3` selects the second and third element. Let’s try this out by selecting the respective rows in a matrix.

```
x[1:3]
```

```
[[ 4.  5.  6.  7.]
 [ 8.  9. 10. 11.]]
<NDArray 2x4 @cpu(0)>
```

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

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

```
[[ 0.  1.  2.  3.]
 [ 4.  5.  9.  7.]
 [ 8.  9. 10. 11.]]
<NDArray 3x4 @cpu(0)>
```

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. 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
```

```
[[12. 12. 12. 12.]
 [12. 12. 12. 12.]
 [ 8.  9. 10. 11.]]
<NDArray 3x4 @cpu(0)>
```

#### 4.1.5 Saving Memory

In the previous example, every time we ran an operation, we allocated new memory to host its results. For example, if we write `y = x + y`, we will dereference the matrix that `y` used to point to and instead point it 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 subsequently redirects `y` to point at 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, this could cause a memory leak, making it possible for us to inadvertently reference stale parameters.

Fortunately, performing in-place operations in MXNet is easy. We can assign the result of an operation to a previously allocated array with slice notation, e.g., `y[:] = <expression>`. To illustrate the behavior, we first clone the shape of a matrix using `zeros_like` to allocate a block of 0 entries.

```
z = y.zeros_like()
print('id(z):', id(z))
z[:] = x + y
print('id(z):', id(z))
```

```
id(z): 139885367805320
id(z): 139885367805320
```

While this looks pretty, `x+y` here will still allocate a temporary buffer to store the result of `x+y` before copying it to `z[:]`. To make even better use of memory, we can directly invoke the underlying `ndarray` operation, in this case `elemwise_add`, avoiding temporary buffers. We do this by specifying the `out` keyword argument, which every `ndarray` operator supports:

```
before = id(z)
nd.elemwise_add(x, y, out=z)
id(z) == before
```

```
True
```

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
```

#### 4.1.6 Mutual Transformation of NDArray and NumPy

Converting MXNet NDArrays to and from NumPy is easy. The converted arrays do *not* share memory. This minor inconvenience is actually quite important: when you perform operations on the CPU or one of the GPUs, you do not want MXNet having to wait whether NumPy might want to be doing something else with the same chunk of memory. The `array` and `asnumpy` functions do the trick.

```
import numpy as np

a = x.asnumpy()
print(type(a))
b = nd.array(a)
print(type(b))
```

```
<class 'numpy.ndarray'>
<class 'mxnet.ndarray.ndarray.NDArray'>
```

#### 4.1.7 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 NDArray you can get.
2. Replace the two NDArrays that operate by element in the broadcast mechanism with other shapes, e.g. three dimensional tensors. Is the result the same as expected?
3. Assume that we have three matrices `a`, `b` and `c`. Rewrite `c = nd.dot(a, b.T) + c` in the most memory efficient manner.

#### 4.1.8 Scan the QR Code to Discuss<sup>39</sup>



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<sup>39</sup> <https://discuss.mxnet.io/t/2316>

## 4.2 Linear Algebra

Now that you can store and manipulate data, let's briefly review the subset of basic linear algebra that you will need to understand most of the models. We will introduce all the basic concepts, the corresponding mathematical notation, and their realization in code all in one place. If you are already confident in your basic linear algebra, feel free to skim through or skip this chapter.

```
from mxnet import nd
```

### 4.2.1 Scalars

If you never studied linear algebra or machine learning, you are probably used to working with one number at a time. And know how to do basic things like add them together or multiply them. For example, in Palo Alto, the temperature is 52 degrees Fahrenheit. Formally, we call these values *scalars*. If you wanted to convert this value to Celsius (using metric system's more sensible unit of temperature measurement), you would evaluate the expression  $c = (f - 32) * 5/9$  setting  $f$  to 52. In this equation, each of the terms 32, 5, and 9 is a scalar value. The placeholders  $c$  and  $f$  that we use are called variables and they represent unknown scalar values.

In mathematical notation, we represent scalars with ordinary lower-cased letters ( $x, y, z$ ). We also denote the space of all scalars as  $\mathcal{R}$ . For expedience, we are going to punt a bit on what precisely a space is, but for now, remember that if you want to say that  $x$  is a scalar, you can simply say  $x \in \mathcal{R}$ . The symbol  $\in$  can be pronounced "in" and just denotes membership in a set.

In MXNet, we work with scalars by creating NDArrays with just one element. In this snippet, we instantiate two scalars and perform some familiar arithmetic operations with them, such as addition, multiplication, division and exponentiation.

```
x = nd.array([3.0])
y = nd.array([2.0])

print('x + y = ', x + y)
print('x * y = ', x * y)
print('x / y = ', x / y)
print('x ** y = ', nd.power(x,y))
```

```
x + y =
[5.]
<NDArray 1 @cpu(0)>
x * y =
[6.]
<NDArray 1 @cpu(0)>
x / y =
[1.5]
<NDArray 1 @cpu(0)>
x ** y =
[9.]
<NDArray 1 @cpu(0)>
```

We can convert any NDArray to a Python float by calling its `asscalar` method. Note that this is typically a bad idea. While you are doing this, NDArray has to stop doing anything else in order to hand the result and the process control back to Python. And unfortunately Python is not very good at doing things in parallel.

So avoid sprinkling this operation liberally throughout your code or your networks will take a long time to train.

```
x.asscalar()
```

```
3.0
```

## 4.2.2 Vectors

You can think of a vector as simply a list of numbers, for example `[1.0, 3.0, 4.0, 2.0]`. Each of the numbers in the vector consists of a single scalar value. We call these values the *entries* or *components* of the vector. Often, we are interested in vectors whose values hold some real-world significance. For example, if we are studying the risk that loans default, we might associate each applicant with a vector whose components correspond to their income, length of employment, number of previous defaults, etc. If we were studying the risk of heart attacks hospital patients potentially face, we might represent each patient with 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 (**u**, **v**, **w**). In MXNet, we work with vectors via 1D NDArrays with an arbitrary number of components.

```
x = nd.arange(4)
print('x = ', x)
```

```
x =
[0. 1. 2. 3.]
<NDArray 4 @cpu(0)>
```

We can refer to any element of a vector by using a subscript. For example, we can refer to the 4th element of **u** by  $u_4$ . Note that the element  $u_4$  is a scalar, so we do not bold-face the font when referring to it. In code, we access any element *i* by indexing into the `NDArray`.

```
x[3]
```

```
[3.]
<NDArray 1 @cpu(0)>
```

## 4.2.3 Length, dimensionality and shape

Let's revisit some concepts from the previous section. 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 **x** consists of *n* real-valued scalars, we can express this as  $\mathbf{x} \in \mathcal{R}^n$ . The length of a vector is commonly called its *dimension*. As with an ordinary Python array, we can access the length of an `NDArray` by calling Python's in-built `len()` function.

We can also access a vector's length via its `.shape` attribute. The shape is a tuple that lists the dimensionality of the `NDArray` along each of its axes. Because a vector can only be indexed along one axis, its shape has just one element.

```
x.shape
```

```
(4,)
```

Note that the word dimension is overloaded and this tends to confuse people. Some use the *dimensionality* of a vector to refer to its length (the number of components). However some use the word *dimensionality* to refer to the number of axes that an array has. In this sense, a scalar *would have* 0 dimensions and a vector *would have* 1 dimension.

To avoid confusion, when we say **2D array** or **3D array**, we mean an array with **2** or **3** axes respectively. But if we say :math:`‘n`-dimensional vector, we mean a vector of length :math:`‘n`.

```
a = 2
x = nd.array([1,2,3])
y = nd.array([10,20,30])
print(a * x)
print(a * x + y)
```

```
[2. 4. 6.]
<NDArray 3 @cpu(0)>

[12. 24. 36.]
<NDArray 3 @cpu(0)>
```

#### 4.2.4 Matrices

Just as vectors generalize scalars from order 0 to order 1, matrices generalize vectors from  $1D$  to  $2D$ . Matrices, which we'll typically denote with capital letters ( $A, B, C$ ), are represented in code as arrays with 2 axes. Visually, we can draw a matrix as a table, where each entry  $a_{ij}$  belongs to the  $i$ -th row and  $j$ -th column.

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{pmatrix} \quad (4.2.1)$$

We can create a matrix with  $n$  rows and  $m$  columns in MXNet by specifying a shape with two components ( $n, m$ ) when calling any of our favorite functions for instantiating an `ndarray` such as `ones`, or `zeros`.

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

```
[[ 0.  1.  2.  3.]
 [ 4.  5.  6.  7.]
 [ 8.  9. 10. 11.]
 [12. 13. 14. 15.]
 [16. 17. 18. 19.]]
<NDArray 5x4 @cpu(0)>
```

Matrices are useful data structures: they allow us to organize data that has different modalities of variation. For example, rows in our matrix might correspond to different patients, while columns might correspond to different attributes.

We can access the scalar elements  $a_{ij}$  of a matrix  $A$  by specifying the indices for the row ( $i$ ) and column ( $j$ ) respectively. Leaving them blank via `a :` takes all elements along the respective dimension (as seen in the previous section).

We can transpose the matrix through `T`. That is, if  $B = A^T$ , then  $b_{ij} = a_{ji}$  for any  $i$  and  $j$ .

```
print(A.T)
```

```
[[ 0.  4.  8. 12. 16.]
 [ 1.  5.  9. 13. 17.]
 [ 2.  6. 10. 14. 18.]
 [ 3.  7. 11. 15. 19.]]
<NDArray 4x5 @cpu(0)>
```

## 4.2.5 Tensors

Just as vectors generalize scalars, and matrices generalize vectors, we can actually build data structures with even more axes. Tensors give us a generic way of discussing arrays with an arbitrary number of axes. Vectors, for example, are first-order tensors, and matrices are second-order tensors.

Using tensors will become more important when we start working with images, which arrive as 3D data structures, with axes corresponding to the height, width, and the three (RGB) color channels. But in this chapter, we're going to skip this part and make sure you know the basics.

```
X = nd.arange(24).reshape((2, 3, 4))
print('X.shape =', X.shape)
print('X =', X)
```

```
X.shape = (2, 3, 4)
X =
[[[ 0.  1.  2.  3.]
 [ 4.  5.  6.  7.]
 [ 8.  9. 10. 11.]]
 [[12. 13. 14. 15.]
 [16. 17. 18. 19.]
 [20. 21. 22. 23.]]]
<NDArray 2x3x4 @cpu(0)>
```

## 4.2.6 Basic properties of tensor arithmetic

Scalars, vectors, matrices, and tensors of any order have some nice properties that we will often rely on. For example, as you might have noticed from the definition of an element-wise operation, given operands with the same shape, the result of any element-wise operation is a tensor of that same shape. Another convenient property is that for all tensors, multiplication by a scalar produces a tensor of the same shape. In math, given two tensors  $X$  and  $Y$  with the same shape,  $\alpha X + Y$  has the same shape (numerical mathematicians call this the AXPY operation).

```
a = 2
x = nd.ones(3)
y = nd.zeros(3)
print(x.shape)
print(y.shape)
print((a * x).shape)
print((a * x + y).shape)
```

```
(3,)  
(3,)  
(3,)  
(3,)
```

Shape is not the only property preserved under addition and multiplication by a scalar. These operations also preserve membership in a vector space. But we will postpone this discussion for the second half of this chapter because it is not critical to getting your first models up and running.

#### 4.2.7 Sums and means

The next more sophisticated thing we can do 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  $\mathbf{u}$  of length  $d$ , we can write  $\sum_{i=1}^d u_i$ . In code, we can just call `nd.sum()`.

```
print(x)
print(nd.sum(x))
```

```
[1. 1. 1.]
<NDArray 3 @cpu(0)>

[3.]
<NDArray 1 @cpu(0)>
```

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

```
print(A)
print(nd.sum(A))
```

```
[[ 0.  1.  2.  3.]
 [ 4.  5.  6.  7.]
 [ 8.  9.  10. 11.]
 [12. 13. 14. 15.]
 [16. 17. 18. 19.]]
<NDArray 5x4 @cpu(0)>

[190.]
<NDArray 1 @cpu(0)>
```

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. With mathematical notation, we could write the average over a vector  $\mathbf{u}$  as  $\frac{1}{d} \sum_{i=1}^d u_i$  and the average over a matrix  $A$  as  $\frac{1}{n \cdot m} \sum_{i=1}^m \sum_{j=1}^n a_{ij}$ . In code, we could just call `nd.mean()` on tensors of arbitrary shape:

```
print(nd.mean(A))
print(nd.sum(A) / A.size)
```

```
[9.5]
<NDArray 1 @cpu(0)>
```

(continues on next page)

(continued from previous page)

```
[9.5]
<NDArray 1 @cpu(0)>
```

## 4.2.8 Dot products

So far, we have only performed element-wise operations, sums and averages. And if this was all we could do, linear algebra probably would not deserve its own chapter. However, one of the most fundamental operations is the dot product. Given two vectors  $\mathbf{u}$  and  $\mathbf{v}$ , the dot product  $\mathbf{u}^T \mathbf{v}$  is a sum over the products of the corresponding elements:  $\mathbf{u}^T \mathbf{v} = \sum_{i=1}^d u_i \cdot v_i$ .

```
x = nd.arange(4)
y = nd.ones(4)
print(x, y, nd.dot(x, y))
```

```
[0. 1. 2. 3.]
<NDArray 4 @cpu(0)>
[1. 1. 1. 1.]
<NDArray 4 @cpu(0)>
[6.]
<NDArray 1 @cpu(0)>
```

Note that we can express the dot product of two vectors `nd.dot(x, y)` equivalently by performing an element-wise multiplication and then a sum:

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

```
[6.]
<NDArray 1 @cpu(0)>
```

Dot products are useful in a wide range of contexts. For example, given a set of weights  $\mathbf{w}$ , the weighted sum of some values  $u$  could be expressed as the dot product  $\mathbf{u}^T \mathbf{w}$ . When the weights are non-negative and sum to one ( $\sum_{i=1}^d w_i = 1$ ), the dot product expresses a *weighted average*. When two vectors each have length one (we will discuss what *length* means below in the section on norms), dot products can also capture the cosine of the angle between them.

## 4.2.9 Matrix-vector products

Now that we know how to calculate dot products we can begin to understand matrix-vector products. Let's start off by visualizing a matrix  $A$  and a column vector  $\mathbf{x}$ .

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix} \quad (4.2.2)$$

We can visualize the matrix in terms of its row vectors

$$A = \begin{pmatrix} \mathbf{a}_1^T \\ \mathbf{a}_2^T \\ \vdots \\ \mathbf{a}_n^T \end{pmatrix}, \quad (4.2.3)$$

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

Then the matrix vector product  $\mathbf{y} = A\mathbf{x}$  is simply a column vector  $\mathbf{y} \in \mathbb{R}^n$  where each entry  $y_i$  is the dot product  $\mathbf{a}_i^T \mathbf{x}$ .

$$A\mathbf{x} = \begin{pmatrix} \mathbf{a}_1^T \\ \mathbf{a}_2^T \\ \vdots \\ \mathbf{a}_n^T \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix} = \begin{pmatrix} \mathbf{a}_1^T \mathbf{x} \\ \mathbf{a}_2^T \mathbf{x} \\ \vdots \\ \mathbf{a}_n^T \mathbf{x} \end{pmatrix} \quad (4.2.4)$$

So you can think of multiplication by a matrix  $A \in \mathbb{R}^{n \times m}$  as a transformation that projects vectors from  $\mathbb{R}^m$  to  $\mathbb{R}^n$ .

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 calculations of each layer in a neural network.

Expressing matrix-vector products in code with `ndarray`, we use the same `nd.dot()` function as for dot products. When we call `nd.dot(A, x)` with a matrix  $A$  and a vector  $x$ , MXNet knows to perform a matrix-vector product. Note that the column dimension of  $A$  must be the same as the dimension of  $x$ .

```
nd.dot(A, x)
```

```
[ 14.  38.  62.  86. 110.]  
<NDArray 5 @cpu(0)>
```

## 4.2.10 Matrix-matrix multiplication

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

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

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nk} \end{pmatrix}, \quad B = \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1m} \\ b_{21} & b_{22} & \cdots & b_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ b_{k1} & b_{k2} & \cdots & b_{km} \end{pmatrix} \quad (4.2.5)$$

To produce the matrix product  $C = AB$ , it's easiest to think of  $A$  in terms of its row vectors and  $B$  in terms of its column vectors:

$$A = \begin{pmatrix} \mathbf{a}_1^T \\ \mathbf{a}_2^T \\ \vdots \\ \mathbf{a}_n^T \end{pmatrix}, \quad B = (\mathbf{b}_1 \ \mathbf{b}_2 \ \cdots \ \mathbf{b}_m). \quad (4.2.6)$$

Note here that each row vector  $\mathbf{a}_i^T$  lies in  $\mathbb{R}^k$  and that each column vector  $\mathbf{b}_j$  also lies in  $\mathbb{R}^k$ .

Then to produce the matrix product  $C \in \mathbb{R}^{n \times m}$  we simply compute each entry  $c_{ij}$  as the dot product  $\mathbf{a}_i^T \mathbf{b}_j$ .

$$C = AB = \begin{pmatrix} \mathbf{a}_1^T \\ \mathbf{a}_2^T \\ \vdots \\ \mathbf{a}_n^T \end{pmatrix} (\mathbf{b}_1 \ \mathbf{b}_2 \ \cdots \ \mathbf{b}_m) = \begin{pmatrix} \mathbf{a}_1^T \mathbf{b}_1 & \mathbf{a}_1^T \mathbf{b}_2 & \cdots & \mathbf{a}_1^T \mathbf{b}_m \\ \mathbf{a}_2^T \mathbf{b}_1 & \mathbf{a}_2^T \mathbf{b}_2 & \cdots & \mathbf{a}_2^T \mathbf{b}_m \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{a}_n^T \mathbf{b}_1 & \mathbf{a}_n^T \mathbf{b}_2 & \cdots & \mathbf{a}_n^T \mathbf{b}_m \end{pmatrix} \quad (4.2.7)$$

You can think of the matrix-matrix multiplication  $AB$  as simply performing  $m$  matrix-vector products and stitching the results together to form an  $n \times m$  matrix. Just as with ordinary dot products and matrix-vector products, we can compute matrix-matrix products in MXNet by using `nd.dot()`.

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

```
[[ 6.  6.  6.]
 [22. 22. 22.]
 [38. 38. 38.]
 [54. 54. 54.]
 [70. 70. 70.]]
<NDArray 5x3 @cpu(0)>
```

## 4.2.11 Norms

Before we can start implementing models, there is one last concept we are going to introduce. Some of the most useful operators in linear algebra are norms. Informally, they tell us how big a vector or matrix is. We represent norms with the notation  $\|\cdot\|$ . The  $\cdot$  in this expression is just a placeholder. For example, we would represent the norm of a vector  $\mathbf{x}$  or matrix  $A$  as  $\|\mathbf{x}\|$  or  $\|A\|$ , respectively.

All norms must satisfy a handful of properties:

1.  $\|\alpha A\| = |\alpha| \|A\|$
2.  $\|A + B\| \leq \|A\| + \|B\|$
3.  $\|A\| \geq 0$
4. If  $\forall i, j, a_{ij} = 0$ , then  $\|A\| = 0$

To put it in words, the first rule says that if we scale all the components of a matrix or vector by a constant factor  $\alpha$ , its norm also scales by the *absolute value* of the same constant factor. The second rule is the familiar triangle inequality. The third rule simply says that the norm must be non-negative. That makes sense, in most contexts the smallest *size* for anything is 0. The final rule basically says that the smallest norm is achieved by a matrix or vector consisting of all zeros. It is possible to define a norm that gives zero norm to nonzero matrices, but you cannot give nonzero norm to zero matrices. That may seem like a mouthful, but if you digest it then you probably have grepped the important concepts here.

If you remember Euclidean distances (think Pythagoras' theorem) from grade school, then non-negativity and the triangle inequality might ring a bell. You might notice that norms sound a lot like measures of distance.

In fact, the Euclidean distance  $\sqrt{x_1^2 + \dots + x_n^2}$  is a norm. Specifically it is the  $\ell_2$ -norm. An analogous computation, performed over the entries of a matrix, e.g.  $\sqrt{\sum_{i,j} a_{ij}^2}$ , is called the Frobenius norm. More often, in machine learning we work with the squared  $\ell_2$  norm (notated  $\ell_2^2$ ). We also commonly work with the  $\ell_1$  norm. The  $\ell_1$  norm is simply the sum of the absolute values. It has the convenient property of placing less emphasis on outliers.

To calculate the  $\ell_2$  norm, we can just call `nd.norm()`.

```
nd.norm(x)
```

```
[3.7416573]
<NDArray 1 @cpu(0)>
```

To calculate the L1-norm we can simply perform the absolute value and then sum over the elements.

```
nd.sum(nd.abs(x))
```

```
[6.]  
<NDArray 1 @cpu(0)>
```

## 4.2.12 Norms and objectives

While we do not want to get too far ahead of ourselves, we do want you to anticipate why these concepts are useful. In machine 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, these objectives, perhaps the most important component of a machine learning algorithm (besides the data itself), are expressed as norms.

## 4.2.13 Intermediate linear algebra

If you have made it this far, and understand everything that we have covered, then honestly, you *are* ready to begin modeling. If you are feeling antsy, this is a perfectly reasonable place to move on. You already know nearly all of the linear algebra required to implement a number of many practically useful models and you can always circle back when you want to learn more.

But there is a lot more to linear algebra, even as concerns machine learning. At some point, if you plan to make a career in machine learning, you will need to know more than what we have covered so far. In the rest of this chapter, we introduce some useful, more advanced concepts.

### Basic vector properties

Vectors are useful beyond being data structures to carry numbers. In addition to reading and writing values to the components of a vector, and performing some useful mathematical operations, we can analyze vectors in some interesting ways.

One important concept is the notion of a vector space. Here are the conditions that make a vector space:

- **Additive axioms** (we assume that  $x, y, z$  are all vectors):  $x + y = y + x$  and  $(x + y) + z = x + (y + z)$  and  $0 + x = x + 0 = x$  and  $(-x) + x = x + (-x) = 0$ .
- **Multiplicative axioms** (we assume that  $x$  is a vector and  $a, b$  are scalars):  $0 \cdot x = 0$  and  $1 \cdot x = x$  and  $(ab)x = a(bx)$ .
- **Distributive axioms** (we assume that  $x$  and  $y$  are vectors and  $a, b$  are scalars):  $a(x + y) = ax + ay$  and  $(a + b)x = ax + bx$ .

### Special matrices

There are a number of special matrices that we will use throughout this tutorial. Let's look at them in a bit of detail:

- **Symmetric Matrix** These are matrices where the entries below and above the diagonal are the same. In other words, we have that  $M^\top = M$ . An example of such matrices are those that describe pairwise distances, i.e.  $M_{ij} = \|x_i - x_j\|$ . Likewise, the Facebook friendship graph can be written as a symmetric

matrix where  $M_{ij} = 1$  if  $i$  and  $j$  are friends and  $M_{ij} = 0$  if they are not. Note that the *Twitter* graph is asymmetric -  $M_{ij} = 1$ , i.e.  $i$  following  $j$  does not imply that  $M_{ji} = 1$ , i.e.  $j$  following  $i$ .

- **Antisymmetric Matrix** These matrices satisfy  $M^\top = -M$ . Note that any square matrix can always be decomposed into a symmetric and into an antisymmetric matrix by using  $M = \frac{1}{2}(M + M^\top) + \frac{1}{2}(M - M^\top)$ .
- **Diagonally Dominant Matrix** These are matrices where the off-diagonal elements are small relative to the main diagonal elements. In particular we have that  $M_{ii} \geq \sum_{j \neq i} M_{ij}$  and  $M_{ii} \geq \sum_{j \neq i} M_{ji}$ . If a matrix has this property, we can often approximate  $M$  by its diagonal. This is often expressed as  $\text{diag}(M)$ .
- **Positive Definite Matrix** These are matrices that have the nice property where  $x^\top M x > 0$  whenever  $x \neq 0$ . Intuitively, they are a generalization of the squared norm of a vector  $\|x\|^2 = x^\top x$ . It is easy to check that whenever  $M = A^\top A$ , this holds since there  $x^\top M x = x^\top A^\top Ax = \|Ax\|^2$ . There is a somewhat more profound theorem which states that all positive definite matrices can be written in this form.

#### 4.2.14 Summary

In just a few pages (or one Jupyter notebook) we have taught you all the linear algebra you will need to understand a good chunk of neural networks. Of course there is a *lot* more to linear algebra. And a lot of that math *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 math much later on, we will wrap up this chapter here.

If you are eager to learn more about linear algebra, here are some of our favorite resources on the topic

- For a solid primer on basics, check out Gilbert Strang's book [Introduction to Linear Algebra](#)<sup>40</sup>
- Zico Kolter's [Linear Algebra Review and Reference](#)<sup>41</sup>

#### 4.2.15 Scan the QR Code to Discuss<sup>42</sup>



### 4.3 Automatic Differentiation

In machine 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?” With neural networks, we typically choose loss functions that are

<sup>40</sup> <http://math.mit.edu/~gs/linearalgebra/>

<sup>41</sup> <http://www.cs.cmu.edu/~zkolter/course/15-884/linalg-review.pdf>

<sup>42</sup> <https://discuss.mxnet.io/t/2317>

differentiable with respect to our parameters. Put simply, this means that for each of the model's parameters, we can determine how much *increasing* or *decreasing* it might affect the loss. 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).

The autograd package expedites this work by automatically calculating derivatives. And while many other libraries require that we compile a symbolic graph to take automatic derivatives, `autograd` allows us to take derivatives while writing ordinary imperative code. Every time we pass data through our model, `autograd` builds a graph on the fly, tracking which data combined through which operations to produce the output. This graph enables `autograd` to subsequently backpropagate gradients on command. Here *backpropagate* simply means to trace through the compute graph, filling in the partial derivatives with respect to each parameter. If you are unfamiliar with some of the math, e.g. gradients, please refer to [Section 17.2](#).

```
from mxnet import autograd, nd
```

### 4.3.1 A Simple Example

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

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

```
[0. 1. 2. 3.]
<NDArray 4 @cpu(0)>
```

Once we compute the gradient of  $y$  with respect to  $\mathbf{x}$ , we will need a place to store it. We can tell an NDArray that we plan to store a gradient by invoking its `attach_grad()` method.

```
x.attach_grad()
```

Now we are going to compute  $y$  and MXNet will generate a computation graph on the fly. It is as if MXNet turned on a recording device and captured the exact path by which each variable was generated.

Note that building the computation graph requires a nontrivial amount of computation. So MXNet will only build the graph when explicitly told to do so. This happens by placing code inside a `with autograd.record():` block.

```
with autograd.record():
    y = 2 * nd.dot(x, x)
y
```

```
[28.]
<NDArray 1 @cpu(0)>
```

Since  $\mathbf{x}$  is a vector of length 4, `nd.dot` will perform inner product and therefore  $y$  is a scalar. Next, we can automatically find the gradient of all the inputs by calling the `backward` function.

```
y.backward()
```

The gradient of the function  $y = 2\mathbf{x}^\top \mathbf{x}$  with respect to  $\mathbf{x}$  should be  $4\mathbf{x}$ . Now let's verify that the gradient produced is correct.

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

```
[0. 0. 0. 0.]  
<NDArray 4 @cpu(0)>
```

If  $x$  is used in another computation to compute the gradient, previous `x.grad` contents will be overwritten.

```
with autograd.record():  
    y = x.norm()  
y.backward()  
x.grad
```

```
[0. 0.26726124 0.5345225 0.80178374]  
<NDArray 4 @cpu(0)>
```

### 4.3.2 Backward for Non-scalar Variable

When  $y$  is not a scalar, the gradients could be high order tensor and complex to compute (refer to Section 17.2). In both machine learning and deep learning, luckily we only compute gradients for loss functions, whose values are often scalars. So MXNet will sum the elements in  $y$  to get the new variable by default, and then find the analytical gradient of the variable with respect to  $x$  evaluated at its current value  $\frac{dy}{dx}$ .

```
with autograd.record(): # y is a vector  
    y = x * x  
y.backward()  
  
u = x.copy()  
u.attach_grad()  
with autograd.record(): # v is scalar  
    v = (u * u).sum()  
v.backward()  
  
x.grad = u.grad
```

```
[0. 0. 0. 0.]  
<NDArray 4 @cpu(0)>
```

### 4.3.3 Detach Computations

We could move some parts of computations out of the computation graph. Assume  $y = f(x)$  and  $z = g(y)$ . Then  $u = y.detach()$  will return a new variable has the same values as  $y$  but forgets how  $u$  is computed. It equals to compute  $u = f(x)$  not within a `autograd.record` scope, namely  $u$  is treated as constant. The following backward computes  $\partial u^2 x / \partial x$  with  $u = x$  instead of  $\partial x^3 / \partial x$ .

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

```
[0. 0. 0. 0.]  
<NDArray 4 @cpu(0)>
```

Since the computation of  $y$  is still recorded, we can call `y.backward()` to get  $\partial y / \partial x = 2x$ .

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

```
[0. 0. 0. 0.]  
<NDArray 4 @cpu(0)>
```

#### 4.3.4 Attach Gradients to Internal Variables

Attaching gradients to a variable  $x$  implicitly calls `x=x.detach()`. If  $x$  is computed based on other variables, this part of computation will not be used in the backward function.

```
y = nd.ones(4) * 2  
y.attach_grad()  
with autograd.record():  
    u = x * y  
    u.attach_grad() # implicitly run u = u.detach()  
    z = u + x  
z.backward()  
x.grad, u.grad, y.grad
```

```
(  
[1. 1. 1. 1.]  
<NDArray 4 @cpu(0)>,  
[1. 1. 1. 1.]  
<NDArray 4 @cpu(0)>,  
[0. 0. 0. 0.]  
<NDArray 4 @cpu(0)>)
```

#### 4.3.5 Head gradients

Detaching allows to breaks the computation into several parts. We could use chain rule Section 17.2 to compute the gradient for the whole computation. Assume  $u = f(x)$  and  $z = g(u)$ , by chain rule we have  $\frac{dz}{dx} = \frac{dz}{du} \frac{du}{dx}$ . To compute  $\frac{dz}{dx}$ , we can first detach  $u$  from the computation and then call `z.backward()` to compute the first term.

```
y = nd.ones(4) * 2  
y.attach_grad()  
with autograd.record():  
    u = x * y  
    v = u.detach() # u still keeps the computation graph  
    v.attach_grad()  
    z = v + x  
z.backward()  
x.grad, y.grad
```

```
(  
[1. 1. 1. 1.]  
<NDArray 4 @cpu(0)>,  
[0. 0. 0. 0.]  
<NDArray 4 @cpu(0)>)
```

Later on we call `u.backward()` to compute the second term, but pass the first term as the head gradients to multiply both terms so that `x.grad` will contain  $\frac{dz}{dx}$  instead of  $\frac{du}{dx}$ .

```
u.backward(v.grad)  
x.grad, y.grad
```

```
(  
[2. 2. 2. 2.]  
<NDArray 4 @cpu(0)>,  
[0. 1. 2. 3.]  
<NDArray 4 @cpu(0)>)
```

#### 4.3.6 Computing the Gradient of Python Control Flow

One benefit of using automatic differentiation is that even if the computational graph of the function contains Python's control flow (such as conditional and loop control), we may still be able to find the gradient of a variable. Consider the following program: It should be emphasized that the number of iterations of the loop (while loop) and the execution of the conditional statement (if statement) depend on the value of the input `b`.

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

Note that the number of iterations of the while loop and the execution of the conditional statement (if then else) depend on the value of `a`. To compute gradients, we need to `record` the calculation, and then call the `backward` function to calculate the gradient.

```
a = nd.random.normal(shape=1)  
a.attach_grad()  
with autograd.record():  
    d = f(a)  
d.backward()
```

Let's analyze the `f` function defined above. As you can see, it is piecewise linear in its input `a`. In other words, for any `a` there exists some constant such that for a given range  $f(a) = g * a$ . Consequently `d / a` allows us to verify that the gradient is correct:

```
print(a.grad == (d / a))
```

```
[1.]
<NDArray 1 @cpu(0)>
```

### 4.3.7 Training Mode and Prediction Mode

As you can see from the above, after calling the `record` function, MXNet will record the operations and calculate the gradient. In addition, `autograd` will also change the running mode from the prediction mode to the training mode by default. This can be viewed by calling the `is_training` function.

```
print(autograd.is_training())
with autograd.record():
    print(autograd.is_training())
```

```
False
True
```

In some cases, the same model behaves differently in the training and prediction modes (e.g. when using neural techniques such as dropout [Section 6.6](#) and batch normalization [Section 9.5](#)). In other cases, some models may store more auxiliary variables to make computing gradients easier. We will cover these differences in detail in later chapters. For now, you do not need to worry about them.

### 4.3.8 Summary

- MXNet provides an `autograd` package to automate the derivation process. To do so, we first attach gradients to variables, record the computation, and then run the backward function.
- We can detach gradients and pass head gradients to the backward function to control the part of the computation will be used in the backward function.
- The running modes of MXNet include the training mode and the prediction mode. We can determine the running mode by `autograd.is_training()`.

### 4.3.9 Exercises

- Try to run `y.backward()` twice.
- 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?
- Redesign an example of finding the gradient of the control flow. Run and analyze the result.
- In a second-price auction (such as in eBay or in computational advertising), the winning bidder pays the second-highest price. Compute the gradient of the final price with respect to the winning bidder's bid using `autograd`. What does the result tell you about the mechanism? If you are curious to learn more about second-price auctions, check out this paper by Edelman, Ostrovski and Schwartz, 2005<sup>43</sup>.
- Why is the second derivative much more expensive to compute than the first derivative?
- Derive the head gradient relationship for the chain rule. If you get stuck, use the “Chain rule” article on Wikipedia<sup>44</sup>.

<sup>43</sup> <https://www.benedelman.org/publications/gsp-060801.pdf>

<sup>44</sup> [https://en.wikipedia.org/wiki/Chain\\_rule](https://en.wikipedia.org/wiki/Chain_rule)

7. Assume  $f(x) = \sin(x)$ . Plot  $f(x)$  and  $\frac{df(x)}{dx}$  on a graph, where you computed the latter without any symbolic calculations, i.e. without exploiting that  $f'(x) = \cos(x)$ .

#### 4.3.10 Scan the QR Code to Discuss<sup>45</sup>



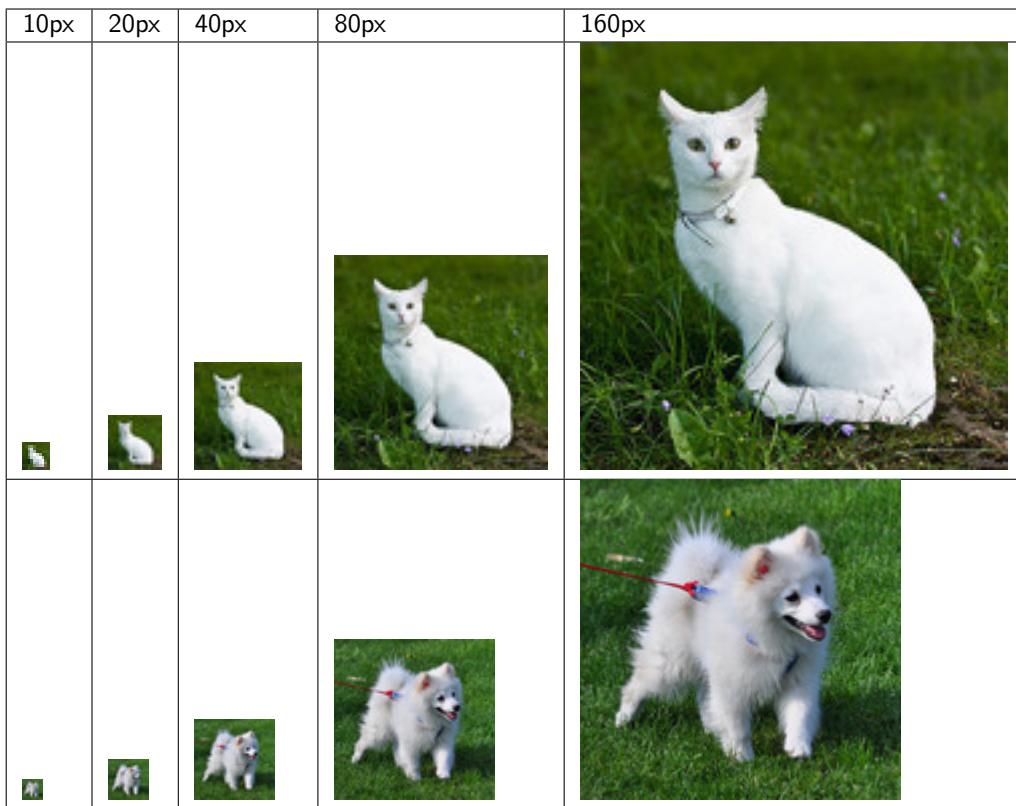
## 4.4 Probability and Statistics

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 action. And when we build recommender systems we also need to think about probability. For example, say *hypothetically* that 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 and statistics. Entire courses, majors, theses, careers, and even departments, are devoted to probability. So naturally, our goal in this section isn't 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 machine 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've already invoked probabilities in previous sections without articulating what precisely they are or giving a concrete example. Let's get more serious now by considering the problem of distinguishing cats and dogs based on photographs. This might sound simple but it's actually a formidable challenge. To start with, the difficulty of the problem may depend on the resolution of the image.

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<sup>45</sup> <https://discuss.mxnet.io/t/2318>



While it's easy for humans to recognize cats and dogs at 320 pixel resolution, it becomes challenging at 40 pixels and next to impossible at 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  $l$  is cat, denoted  $P(l = \text{cat})$  equals 1.0. If we had no evidence to suggest that  $l = \text{cat}$  or that  $l = \text{dog}$ , then we might say that the two possibilities were equally *likely* expressing this as  $P(l = \text{cat}) = 0.5$ . If we were reasonably confident, but not sure that the image depicted a cat, we might assign a probability  $.5 < P(l = \text{cat}) < 1.0$ .

Now consider a second case: given some weather monitoring data, we want to predict the probability that it will rain in Taipei tomorrow. If it's summertime, the rain might come with probability .5. In both cases, we have some value of interest. And in both cases we are uncertain about the outcome. But there's a key difference between the two cases. In this first case, the image is in fact either a dog or a cat, we just don't 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.

#### 4.4.1 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 six outcomes  $\mathcal{X} = \{1, \dots, 6\}$  are equally likely to occur, and thus we would see a 1 in 1 out of 6 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'll observe a value  $\{1, 2, \dots, 6\}$ . 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's going here, let's try it out.

To start, let's import the necessary packages:

```
%matplotlib inline
from IPython import display
import numpy as np
from mxnet import nd
import math
from matplotlib import pyplot as plt
import random
```

Next, we'll want to be able to cast the die. In statistics we call this process of drawing examples from probability distributions *sampling*. The distribution which assigns probabilities to a number of discrete choices is called the *multinomial* distribution. We'll give a more formal definition of *distribution* later, but at a high level, think of it as just an assignment of probabilities to events. In MXNet, we can sample from the multinomial distribution via the aptly named `nd.random.multinomial` function. The function can be called in many ways, but we'll focus on the simplest. To draw a single sample, we simply pass in a vector of probabilities.

```
probabilities = nd.ones(6) / 6
nd.random.multinomial(probabilities)
```

```
[3]
<NDArray 1 @cpu(0)>
```

If you run the sampler a bunch of times, you'll 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 `random.multinomial` supports drawing multiple samples at once, returning an array of independent samples in any shape we might desire.

```
print(nd.random.multinomial(probabilities, shape=(10)))
print(nd.random.multinomial(probabilities, shape=(5,10)))
```

```
[3 4 5 3 5 3 5 2 3 3]
<NDArray 10 @cpu(0)>

[[2 2 1 5 0 5 1 2 2 4]
 [4 3 2 3 2 5 5 0 2 0]
 [3 0 2 4 5 4 0 5 5 5]
 [2 4 4 2 3 4 4 0 4 3]
 [3 0 3 5 4 3 0 2 2 1]]
<NDArray 5x10 @cpu(0)>
```

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.

```
rolls = nd.random.multinomial(probabilities, shape=(1000))
counts = nd.zeros((6,1000))
totals = nd.zeros(6)
for i, roll in enumerate(rolls):
```

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```
totals[int(roll.asscalar())] += 1
counts[:, i] = totals
```

To start, we can inspect the final tally at the end of 1000 rolls.

```
totals / 1000
```

```
[0.167 0.168 0.175 0.159 0.158 0.173]
<NDArray 6 @cpu(0)>
```

As you can see, the lowest estimated probability for any of the numbers is about .15 and the highest estimated probability is 0.188. Because we generated the data from a fair die, we know that each number actually has probability of 1/6, roughly .167, so these estimates are pretty good. We can also visualize how these probabilities converge over time towards reasonable estimates.

To start let's take a look at the `counts` array which has shape (6, 1000). For each time step (out of 1000), `counts` says how many times each of the numbers has shown up. So we can normalize each  $j$ -th column of the counts vector by the number of tosses to give the `current` estimated probabilities at that time. The `counts` object looks like this:

```
counts
```

```
[[ 0.  0.  0. ... 165. 166. 167.]
 [ 1.  1.  1. ... 168. 168. 168.]
 [ 0.  0.  0. ... 175. 175. 175.]
 [ 0.  0.  0. ... 159. 159. 159.]
 [ 0.  1.  2. ... 158. 158. 158.]
 [ 0.  0.  0. ... 173. 173. 173.]]
<NDArray 6x1000 @cpu(0)>
```

Normalizing by the number of tosses, we get:

```
x = nd.arange(1000).reshape((1,1000)) + 1
estimates = counts / x
print(estimates[:,0])
print(estimates[:,1])
print(estimates[:,100])
```

```
[0. 1. 0. 0. 0. 0.]
<NDArray 6 @cpu(0)>

[0. 0.5 0. 0. 0.5 0. ]
<NDArray 6 @cpu(0)>

[0.1980198 0.15841584 0.17821783 0.18811882 0.12871288 0.14851485]
<NDArray 6 @cpu(0)>
```

As you can see, after the first toss of the die, we get the extreme estimate that one of the numbers will be rolled with probability 1.0 and that the others have probability 0. After 100 rolls, things already look a bit more reasonable. We can visualize this convergence.

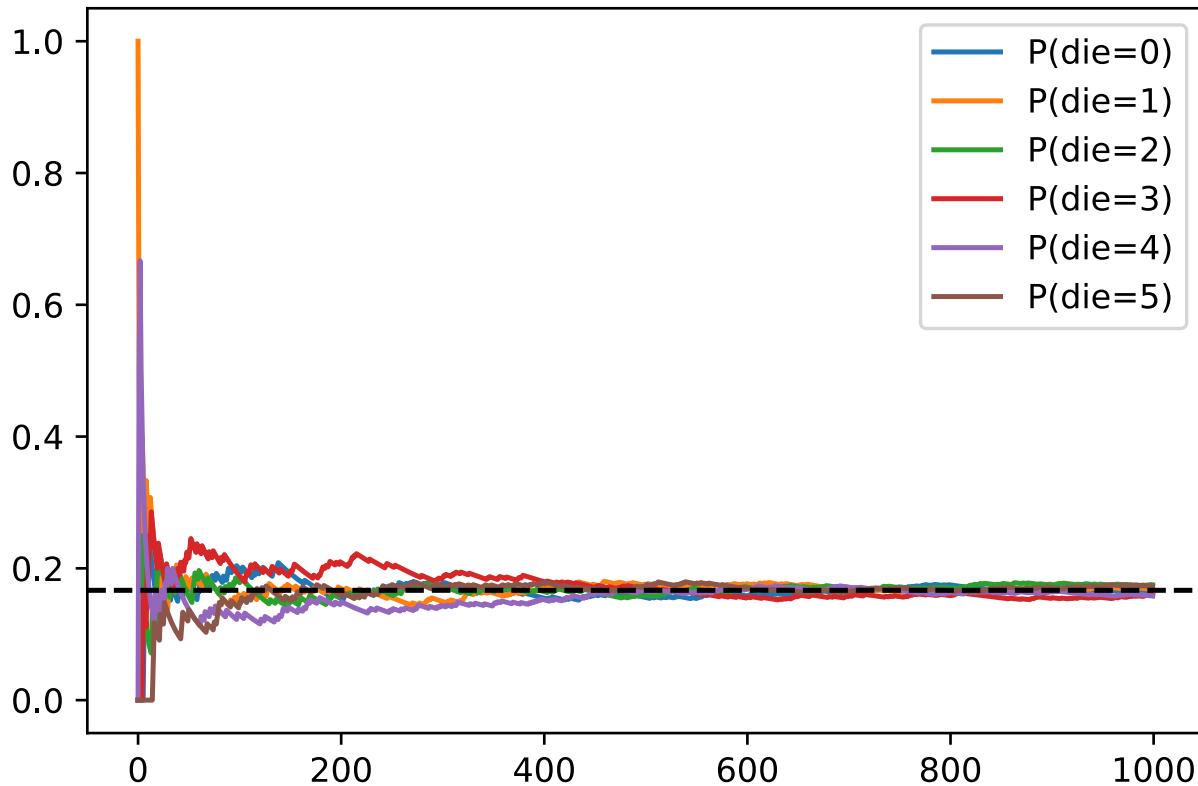
First we define a function that specifies `matplotlib` to output the SVG figures for sharper images, and another one to specify the figure sizes.

```
# Save to the d2l package.
def use_svg_display():
    """Use the svg format to display plot in jupyter."""
    display.set_matplotlib_formats('svg')

# Save to the d2l package.
def set_figsize(figsize=(3.5, 2.5)):
    """Change the default figure size"""
    use_svg_display()
    plt.rcParams['figure.figsize'] = figsize
```

Now visualize the data.

```
set_figsize((6, 4))
for i in range(6):
    plt.plot(estimate[i, :].asnumpy(), label="P(die=" + str(i) + ")")
plt.axhline(y=0.16666, color='black', linestyle='dashed')
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 of the 1000 turns. The dashed black line gives the true underlying probability. As we get more data, the solid curves converge towards the true answer.

In our example of casting a die, we introduced the notion of a **random variable**. A random variable, which we denote here as  $X$  can be pretty much any quantity and is not deterministic. Random variables could take one value among a set of possibilities. We denote sets with brackets, e.g.,  $\{\text{cat}, \text{dog}, \text{rabbit}\}$ . The items contained in the set are called *elements*, and we can say that an element  $x$  is *in* the set  $S$ , by writing

$x \in S$ . The symbol  $\in$  is read as “in” and denotes membership. For instance, we could truthfully say  $\text{dog} \in \{\text{cat}, \text{dog}, \text{rabbit}\}$ . When dealing with the rolls of die, we are concerned with a variable  $X \in \{1, 2, 3, 4, 5, 6\}$ .

Note that there is a subtle difference between discrete random variables, like the sides of a dice, and continuous ones, like the weight and the height of a person. There’s little point in asking whether two people have exactly the same height. If we take precise enough measurements you’ll 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’s no purpose in asking about the probability that someone is 2.00139278291028719210196740527486202 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 1.99 and 2.01 meters. In these cases we quantify the likelihood that we see a value as a *density*. The height of exactly 2.0 meters has no probability, but nonzero density. In the interval between any two different heights we have nonzero probability.

There are a few important axioms of probability that you’ll want to remember:

- For any event  $z$ , the probability is never negative, i.e.  $\Pr(Z = z) \geq 0$ .
- For any two events  $Z = z$  and  $X = x$  the union is no more likely than the sum of the individual events, i.e.  $\Pr(Z = z \cup X = x) \leq \Pr(Z = z) + \Pr(X = x)$ .
- For any random variable, the probabilities of all the values it can take must sum to 1, i.e.  $\sum_{i=1}^n \Pr(Z = z_i) = 1$ .
- For any two *mutually exclusive* events  $Z = z$  and  $X = x$ , the probability that either happens is equal to the sum of their individual probabilities, that is  $\Pr(Z = z \cup X = x) = \Pr(Z = z) + \Pr(X = x)$ .

#### 4.4.2 Dealing with multiple random variables

Very often, we’ll 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 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, camera type, etc. All of these are random variables that occur jointly. When we deal with multiple random variables, there are several quantities of interest. The first is called the joint distribution  $\Pr(A, B)$ . Given any elements  $a$  and  $b$ , the joint distribution lets us answer, what is the probability that  $A = a$  and  $B = b$  simultaneously? Note that for any values  $a$  and  $b$ ,  $\Pr(A = a, B = b) \leq \Pr(A = a)$ .

This has to be the case, since for  $A$  and  $B$  to happen,  $A$  has to happen *and*  $B$  also has to happen (and vice versa). Thus  $A, B$  cannot be more likely than  $A$  or  $B$  individually. This brings us to an interesting ratio:  $0 \leq \frac{\Pr(A, B)}{\Pr(A)} \leq 1$ . We call this a **conditional probability** and denote it by  $\Pr(B|A)$ , the probability that  $B$  happens, provided that  $A$  has happened.

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 that  $\Pr(A, B) = \Pr(B|A) \Pr(A)$ . By symmetry, this also holds for  $\Pr(A, B) = \Pr(A|B) \Pr(B)$ . Solving for one of the conditional variables we get:

$$\Pr(A|B) = \frac{\Pr(B|A) \Pr(A)}{\Pr(B)} \quad (4.4.1)$$

This is very useful if we want to infer one thing from another, say cause and effect but we only know the properties in the reverse direction. One important operation that we need, to make this work, is **marginalization**, i.e., the operation of determining  $\Pr(A)$  and  $\Pr(B)$  from  $\Pr(A, B)$ . We can see that the probability of seeing  $A$  amounts to accounting for all possible choices of  $B$  and aggregating the joint probabilities over all of them, i.e.

$$\Pr(A) = \sum_{B'} \Pr(A, B') \text{ and } \Pr(B) = \sum_{A'} \Pr(A', B) \quad (4.4.2)$$

Another useful property to check for is **dependence** vs. **independence**. Independence is when the occurrence of one event does not reveal any information about the occurrence of the other. In this case  $\Pr(B|A) = \Pr(B)$ . Statisticians typically express this as  $A \perp\!\!\!\perp B$ . From Bayes' Theorem, it follows immediately that also  $\Pr(A|B) = \Pr(A)$ . In all other cases we call  $A$  and  $B$  dependent. For instance, two successive rolls of a die are independent. On the other hand, the position of a light switch and the brightness in the room are not (they are not perfectly deterministic, though, since we could always have a broken lightbulb, power failure, or a broken switch).

Let's put our skills to the test. Assume that a doctor administers an AIDS test to a patient. This test is fairly accurate and it fails only with 1% probability if the patient is healthy by reporting him as diseased. Moreover, it never fails to detect HIV if the patient actually has it. We use  $D$  to indicate the diagnosis and  $H$  to denote the HIV status. Written as a table the outcome  $\Pr(D|H)$  looks as follows:

outcome	HIV positive	HIV negative
Test positive	1	0.01
Test negative	0	0.99

Note that the column sums are all one (but the row sums aren't), since the conditional probability needs to sum up to 1, just like the probability. Let us work out the probability of the patient having AIDS if the test comes back positive. Obviously this is going to depend on how common the disease is, since it affects the number of false alarms. Assume that the population is quite healthy, e.g.  $\Pr(\text{HIV positive}) = 0.0015$ . To apply Bayes' Theorem, we need to determine

$$\begin{aligned} \Pr(\text{Test positive}) &= \Pr(D = 1|H = 0)\Pr(H = 0) + \Pr(D = 1|H = 1)\Pr(H = 1) \\ &= 0.01 \cdot 0.9985 + 1 \cdot 0.0015 \\ &= 0.011485 \end{aligned} \quad (4.4.3)$$

Thus, we get

$$\begin{aligned} \Pr(H = 1|D = 1) &= \frac{\Pr(D = 1|H = 1)\Pr(H = 1)}{\Pr(D = 1)} \\ &= \frac{1 \cdot 0.0015}{0.011485} \\ &= 0.131 \end{aligned} \quad (4.4.4)$$

In other words, there's only a 13.1% chance that the patient actually has AIDS, despite using a test that is 99% accurate. As we can see, statistics can be quite counterintuitive.

### 4.4.3 Conditional independence

What should a patient do upon receiving such terrifying news? Likely, he/she would ask the physician to administer another test to get clarity. The second test has different characteristics (it isn't as good as the first one).

outcome	HIV positive	HIV negative
Test positive	0.98	0.03
Test negative	0.02	0.97

Unfortunately, the second test comes back positive, too. Let us work out the requisite probabilities to invoke Bayes' Theorem.

- $\Pr(D_1 = 1 \text{ and } D_2 = 1 | H = 0) = 0.01 \cdot 0.03 = 0.0003$
- $\Pr(D_1 = 1 \text{ and } D_2 = 1 | H = 1) = 1 \cdot 0.98 = 0.98$
- $\Pr(D_1 = 1 \text{ and } D_2 = 1) = 0.0003 \cdot 0.9985 + 0.98 \cdot 0.0015 = 0.00176955$
- $\Pr(H = 1 | D_1 = 1 \text{ and } D_2 = 1) = \frac{0.98 \cdot 0.0015}{0.00176955} = 0.831$

That is, the second test allowed us to gain much higher confidence that not all is well. Despite the second test being considerably less accurate than the first one, it still improved our estimate quite a bit. You might ask, *why couldn't we just run the first test a second time?* After all, the first test was more accurate. The reason is that we needed a second test whose result is *independent* of the first test (given the true diagnosis). In other words, we made the tacit assumption that  $\Pr(D_1, D_2 | H) = \Pr(D_1 | H) \Pr(D_2 | H)$ . Statisticians call such random variables **conditionally independent**. This is expressed as  $D_1 \perp\!\!\!\perp D_2 | H$ .

#### 4.4.4 Sampling

Often, when working with probabilistic models, we'll want not just to estimate distributions from data, but also to generate data by sampling from distributions. One of the simplest ways to sample random numbers is to invoke the `random` method from Python's `random` package.

```
for i in range(10):
    print(random.random())
```

```
0.1570139994051697
0.0987288794469029
0.33925571612267924
0.8987282702190328
0.5493732669190913
0.4864776413145546
0.8101306859659877
0.05078078452253221
0.6570040380749341
0.30662751360894225
```

#### Uniform Distribution

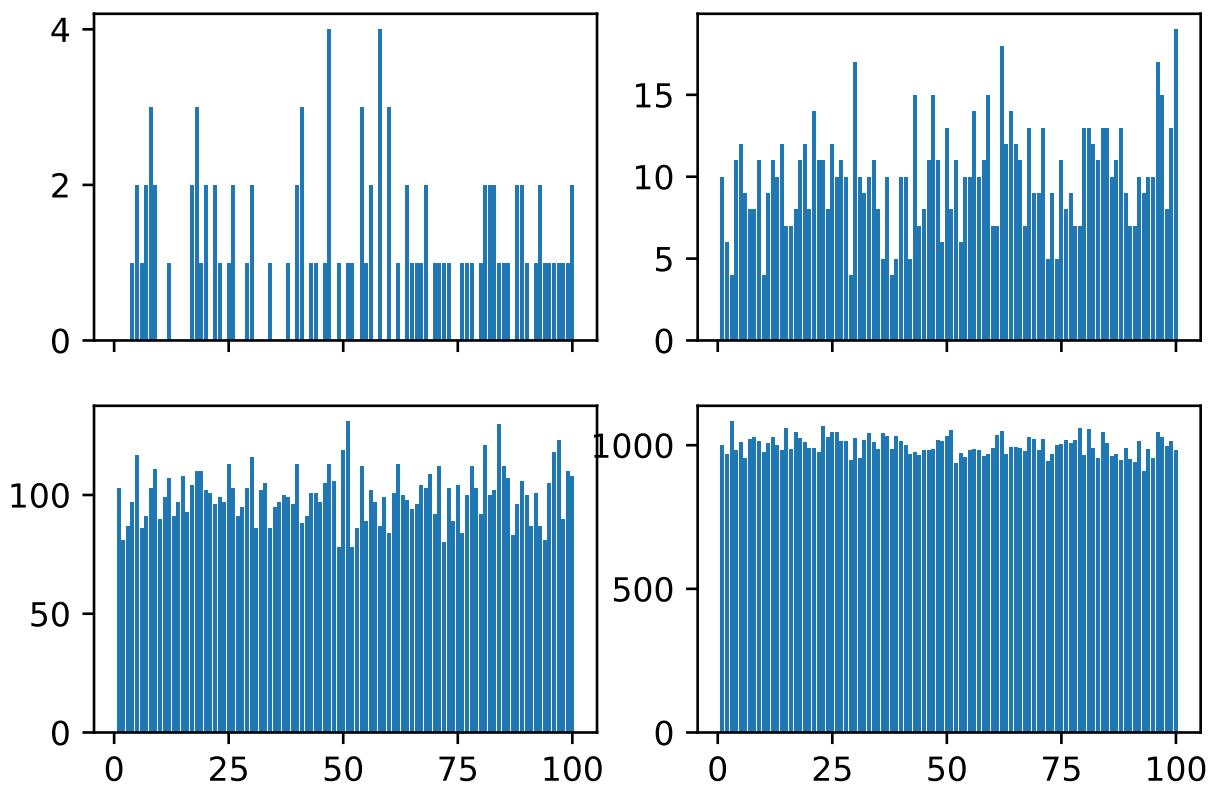
These numbers likely *appear* random. Note that their range is between 0 and 1 and they are evenly distributed. Because these numbers are generated by default from the uniform distribution, there should be no two sub-intervals of  $[0, 1]$  of equal size where numbers are more likely to lie in one interval than the other. In other words, the chances of any of these numbers to fall into the interval  $[0.2, 0.3]$  are the same as in the interval  $[.593264, .693264]$ . In fact, these numbers are pseudo-random, and the computer generates them by first producing a random integer and then dividing it by its maximum range. To sample random integers directly, we can run the following snippet, which generates integers in the range between 1 and 100.

```
for i in range(10):
    print(random.randint(1, 100))
```

```
87
47
39
46
29
33
57
55
80
22
```

How might we check that `randint` is really uniform? Intuitively, the best strategy would be to run sampler many times, say 1 million, and then count the number of times it generates each value to ensure that the results are approximately uniform.

```
counts = np.zeros(100)
fig, axes = plt.subplots(2, 2, sharex=True)
axes = axes.flatten()
# Mangle subplots such that we can index them in a linear fashion rather than
# a 2D grid
for i in range(1, 100001):
    counts[random.randint(0, 99)] += 1
    if i in [100, 1000, 10000, 100000]:
        axes[int(math.log10(i))-2].bar(np.arange(1, 101), counts)
```



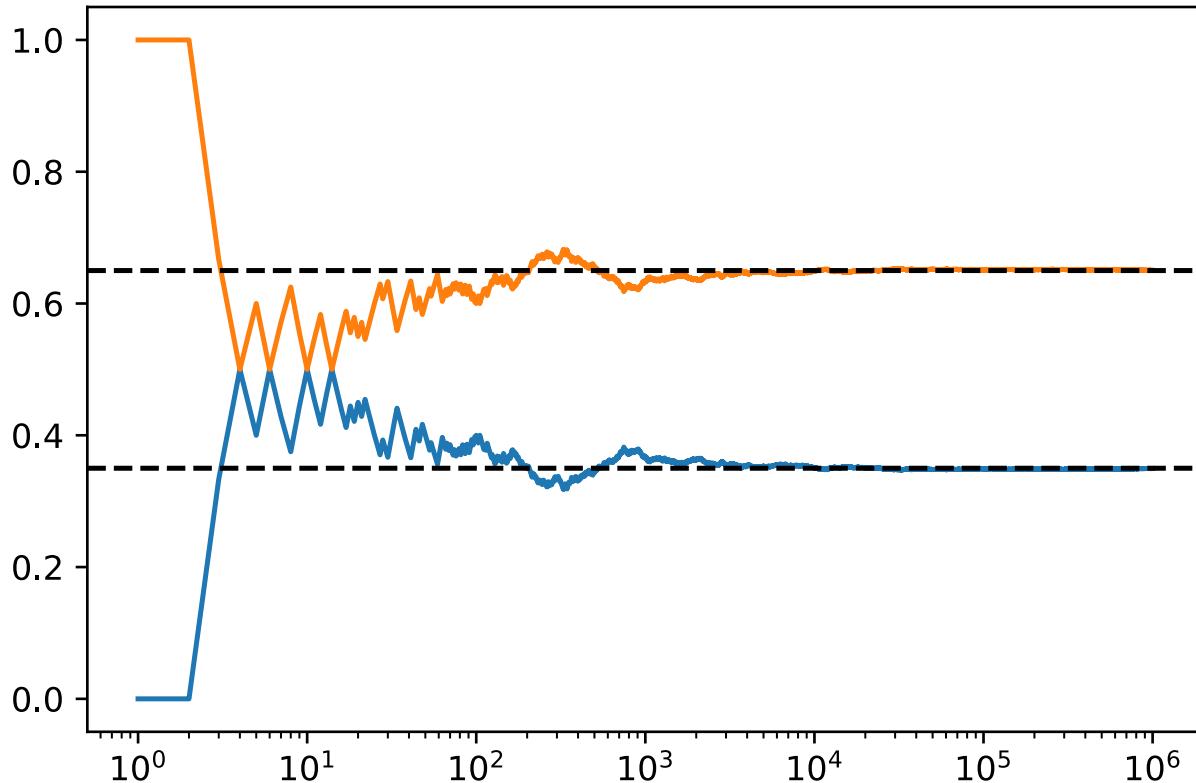
We can see from these figures that the initial number of counts looks *strikingly* uneven. If we sample fewer than 100 draws from a distribution over 100 outcomes this should be expected. But even for 1000 samples there is a significant variability between the draws. What we are really aiming for is a situation where the probability of drawing a number  $x$  is given by  $p(x)$ .

### The categorical distribution

Drawing from a uniform distribution over a set of 100 outcomes is simple. But what if we have nonuniform probabilities? Let's start with a simple case, a biased coin which comes up heads with probability 0.35 and tails with probability 0.65. A simple way to sample from that is to generate a uniform random variable over  $[0, 1]$  and if the number is less than 0.35, we output heads and otherwise we generate tails. Let's try this out.

```
# Number of samples
n = 1000000
y = np.random.uniform(0, 1, n)
x = np.arange(1, n+1)
# Count number of occurrences and divide by the number of total draws
p0 = np.cumsum(y < 0.35) / x
p1 = np.cumsum(y >= 0.35) / x

plt.semilogx(x, p0)
plt.semilogx(x, p1)
plt.axhline(y=0.35, color='black', linestyle='dashed')
plt.axhline(y=0.65, color='black', linestyle='dashed');
```



As we can see, on average, this sampler will generate 35% zeros and 65% ones. Now what if we have more than two possible outcomes? We can simply generalize this idea as follows. Given any probability distribution, e.g.  $p = [0.1, 0.2, 0.05, 0.3, 0.25, 0.1]$  we can compute its cumulative distribution (python's `cumsum` will do this for you)  $F = [0.1, 0.3, 0.35, 0.65, 0.9, 1]$ . Once we have this we draw a random variable  $x$  from the uniform distribution  $U[0, 1]$  and then find the interval where  $F[i - 1] \leq x < F[i]$ . We then return  $i$  as the sample. By construction, the chances of hitting interval  $[F[i - 1], F[i]]$  has probability  $p(i)$ .

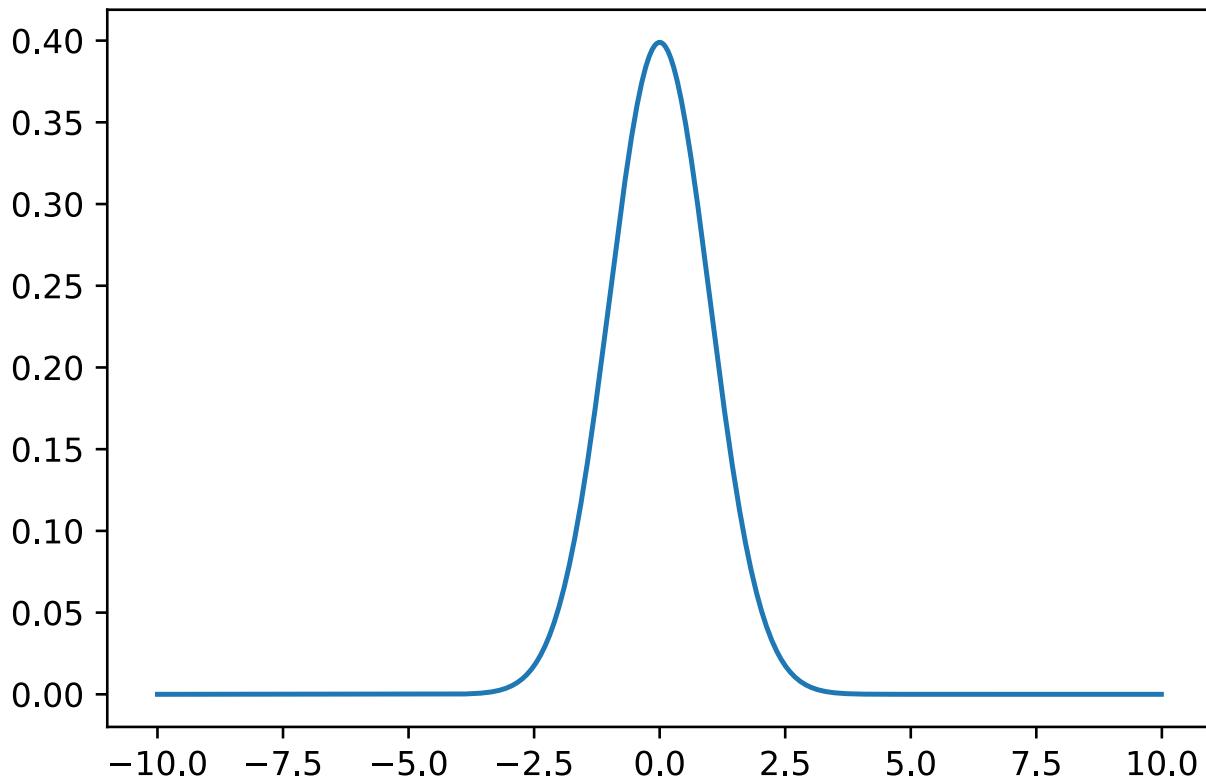
Note that there are many more efficient algorithms for sampling than the one above. For instance, binary search over  $F$  will run in  $O(\log n)$  time for  $n$  random variables. There are even more clever algorithms, such as the [Alias Method](#)<sup>46</sup> to sample in constant time, after  $O(n)$  preprocessing.

### The Normal distribution

The standard Normal distribution (aka the standard Gaussian distribution) is given by  $p(x) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2}x^2)$ . Let's plot it to get a feel for it.

```
x = np.arange(-10, 10, 0.01)
p = (1/math.sqrt(2 * math.pi)) * np.exp(-0.5 * x**2)
plt.plot(x, p);
```

<sup>46</sup> [https://en.wikipedia.org/wiki/Alias\\_method](https://en.wikipedia.org/wiki/Alias_method)



Sampling from this distribution is less trivial. First off, the support is infinite, that is, for any  $x$  the density  $p(x)$  is positive. Secondly, the density is nonuniform. There are many tricks for sampling from it - the key idea in all algorithms is to stratify  $p(x)$  in such a way as to map it to the uniform distribution  $U[0, 1]$ . One way to do this is with the probability integral transform.

Denote by  $F(x) = \int_{-\infty}^x p(z)dz$  the cumulative distribution function (CDF) of  $p$ . This is in a way the continuous version of the cumulative sum that we used previously. In the same way we can now define the inverse map  $F^{-1}(\xi)$ , where  $\xi$  is drawn uniformly. Unlike previously where we needed to find the correct interval for the vector  $F$  (i.e. for the piecewise constant function), we now invert the function  $F(x)$ .

In practice, this is slightly more tricky since inverting the CDF is hard in the case of a Gaussian. It turns out that the *twodimensional* integral is much easier to deal with, thus yielding two normal random variables than one, albeit at the price of two uniformly distributed ones. For now, suffice it to say that there are built-in algorithms to address this.

The normal distribution has yet another desirable property. In a way all distributions converge to it, if we only average over a sufficiently large number of draws from any other distribution. To understand this in a bit more detail, we need to introduce three important things: expected values, means and variances.

- The expected value  $\mathbf{E}_{x \sim p(x)}[f(x)]$  of a function  $f$  under a distribution  $p$  is given by the integral  $\int_x p(x)f(x)dx$ . That is, we average over all possible outcomes, as given by  $p$ .
- A particularly important expected value is that for the function  $f(x) = x$ , i.e.  $\mu := \mathbf{E}_{x \sim p(x)}[x]$ . It provides us with some idea about the typical values of  $x$ .
- Another important quantity is the variance, i.e. the typical deviation from the mean  $\sigma^2 := \mathbf{E}_{x \sim p(x)}[(x - \mu)^2]$ . Simple math shows (check it as an exercise) that  $\sigma^2 = \mathbf{E}_{x \sim p(x)}[x^2] - \mathbf{E}_{x \sim p(x)}^2[x]$ .

The above allows us to change both mean and variance of random variables. Quite obviously for some random variable  $x$  with mean  $\mu$ , the random variable  $x + c$  has mean  $\mu + c$ . Moreover,  $\gamma x$  has the variance  $\gamma^2 \sigma^2$ . Applying this to the normal distribution we see that one with mean  $\mu$  and variance  $\sigma^2$  has the form

$p(x) = \frac{1}{\sqrt{2\sigma^2\pi}} \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right)$ . Note the scaling factor  $\frac{1}{\sigma}$ —it arises from the fact that if we stretch the distribution by  $\sigma$ , we need to lower it by  $\frac{1}{\sigma}$  to retain the same probability mass (i.e. the weight under the distribution always needs to integrate out to 1).

Now we are ready to state one of the most fundamental theorems in statistics, the [Central Limit Theorem](#)<sup>47</sup>. It states that for sufficiently well-behaved random variables, in particular random variables with well-defined mean and variance, the sum tends toward a normal distribution. To get some idea, let's repeat the experiment described in the beginning, but now using random variables with integer values of  $\{0, 1, 2\}$ .

```
# Generate 10 random sequences of 10,000 uniformly distributed random variables
tmp = np.random.uniform(size=(10000,10))
x = 1.0 * (tmp > 0.3) + 1.0 * (tmp > 0.8)
mean = 1 * 0.5 + 2 * 0.2
variance = 1 * 0.5 + 4 * 0.2 - mean**2
print('mean {}, variance {}'.format(mean, variance))

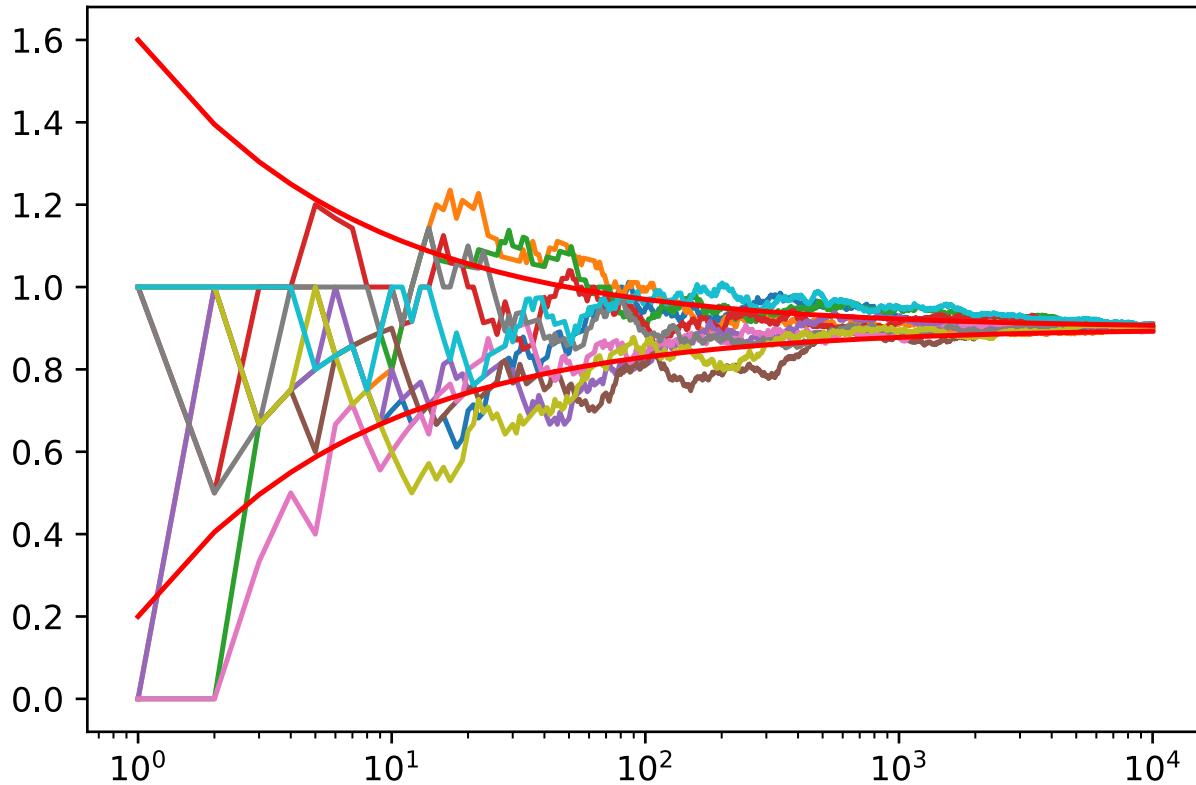
# Cumulative sum and normalization
y = np.arange(1,10001).reshape(10000,1)
z = np.cumsum(x, axis=0) / y

for i in range(10):
    plt.semilogx(y,z[:,i])

plt.semilogx(y,(variance**0.5) * np.power(y,-0.5) + mean,'r')
plt.semilogx(y,-(variance**0.5) * np.power(y,-0.5) + mean,'r');
```

```
mean 0.9, variance 0.49
```

<sup>47</sup> [https://en.wikipedia.org/wiki/Central\\_limit\\_theorem](https://en.wikipedia.org/wiki/Central_limit_theorem)



This looks very similar to the initial example, at least in the limit of averages of large numbers of variables. This is confirmed by theory. Denote by mean and variance of a random variable the quantities

$$\mu[p] := \mathbf{E}_{x \sim p(x)}[x] \text{ and } \sigma^2[p] := \mathbf{E}_{x \sim p(x)}[(x - \mu[p])^2] \quad (4.4.5)$$

Then we have that  $\lim_{n \rightarrow \infty} \frac{1}{\sqrt{n}} \sum_{i=1}^n \frac{x_i - \mu}{\sigma} \rightarrow \mathcal{N}(0, 1)$ . In other words, regardless of what we started out with, we will always converge to a Gaussian. This is one of the reasons why Gaussians are so popular in statistics.

### More distributions

Many more useful distributions exist. If you're interested in going deeper, we recommend consulting a dedicated book on statistics or looking up some common distributions on Wikipedia for further detail. Some important distributions to be aware of include:

- **Binomial Distribution** It is used to describe the distribution over multiple draws from the same distribution, e.g. the number of heads when tossing a biased coin (i.e. a coin with probability  $\pi \in [0, 1]$  of returning heads) 10 times. The binomial probability is given by  $p(x) = \binom{n}{x} \pi^x (1 - \pi)^{n-x}$ .
- **Multinomial Distribution** Often, we are concerned with more than two outcomes, e.g. when rolling a dice multiple times. In this case, the distribution is given by  $p(x) = \frac{n!}{\prod_{i=1}^k x_i!} \prod_{i=1}^k \pi_i^{x_i}$ .
- **Poisson Distribution** This distribution models the occurrence of point events that happen with a given rate, e.g. the number of raindrops arriving within a given amount of time in an area (weird fact - the number of Prussian soldiers being killed by horses kicking them followed that distribution). Given a rate  $\lambda$ , the number of occurrences is given by  $p(x) = \frac{1}{x!} \lambda^x e^{-\lambda}$ .
- **Beta, Dirichlet, Gamma, and Wishart Distributions** They are what statisticians call *conjugate* to the Binomial, Multinomial, Poisson and Gaussian respectively. Without going into detail, these

distributions are often used as priors for coefficients of the latter set of distributions, e.g. a Beta distribution as a prior for modeling the probability for binomial outcomes.

#### 4.4.5 Summary

So far, we covered probabilities, independence, conditional independence, and how to use this to draw some basic conclusions. We also introduced some fundamental probability distributions and demonstrated how to sample from them using Apache MXNet. This is already a powerful bit of knowledge, and by itself a sufficient set of tools for developing some classic machine learning models. In the next section, we will see how to operationalize this knowlege to build your first machine learning model: the Naive Bayes classifier.

#### 4.4.6 Exercises

1. Given two events with probability  $\Pr(A)$  and  $\Pr(B)$ , compute upper and lower bounds on  $\Pr(A \cup B)$  and  $\Pr(A \cap B)$ . Hint - display the situation using a [Venn Diagram](#)<sup>48</sup>.
2. Assume that we have a sequence of events, say  $A$ ,  $B$  and  $C$ , where  $B$  only depends on  $A$  and  $C$  only on  $B$ , can you simplify the joint probability? Hint - this is a [Markov Chain](#)<sup>49</sup>.

#### 4.4.7 Scan the QR Code to Discuss<sup>50</sup>



Fig. 4.4.1: qr

### 4.5 Naive Bayes Classification

Before we worry about complex optimization algorithms or GPUs, we can already deploy our first classifier, relying only on simple statistical estimators and our understanding of conditional independence. Learning is all about making assumptions. If we want to classify a new data point that we've never seen before we have to make some assumptions about which data points are similar to each other. The naive Bayes classifier, a popular and remarkably simple algorithm, assumes all features are independent of each other to simplify the computation. In this chapter, we will apply this model to recognize characters in images.

Let's first import libraries and modules. Especially, we import `d2l`, which now contains the function `use_svg_display` we defined in Section 4.4.

```
%matplotlib inline
import d2l
import math
```

(continues on next page)

<sup>48</sup> [https://en.wikipedia.org/wiki/Venn\\_diagram](https://en.wikipedia.org/wiki/Venn_diagram)

<sup>49</sup> [https://en.wikipedia.org/wiki/Markov\\_chain](https://en.wikipedia.org/wiki/Markov_chain)

<sup>50</sup> <https://discuss.mxnet.io/t/2319>

(continued from previous page)

```
from mxnet import nd, gluon
d2l.use_svg_display()
```

### 4.5.1 Optical Character Recognition

MNIST [34] is one of widely used datasets. It contains 60,000 images for training and 10,000 images for validation. We will formally introduce training data in [Section 5.1](#) and validation data in [Section 6.4](#) later, here we just simply remember we will train the naive Bayes model in the training data and then test its quality on the validation data. Each image contains a handwritten digit from 0 to 9. The task is classifying each image into the corresponding digit.

Gluon, MXNet's high-level interface for implementing neural networks, provides a MNIST class in the `data.vision` module to automatically retrieve the dataset via our Internet connection. Subsequently, Gluon will use the already-downloaded local copy. We specify whether we are requesting the training set or the test set by setting the value of the parameter `train` to `True` or `False`, respectively. Each image is a grayscale image with both width and height of 28 with shape  $(28, 28, 1)$ . We use a customized transformation to remove the last channel dimension. In addition, each pixel is presented by a unsigned 8-bit integer, we quantize them into binary features to simplify the problem.

```
def transform(data, label):
    return nd.floor(data/128).astype('float32').squeeze(axis=-1), label

mnist_train = gluon.data.vision.MNIST(train=True, transform=transform)
mnist_test = gluon.data.vision.MNIST(train=False, transform=transform)
```

We can access a particular example, which contains the image and the corresponding label.

```
image, label = mnist_train[2]
image.shape, label
```

```
((28, 28), 4)
```

Our example, stored here in the variable `image` corresponds to an image with a height and width of 28 pixels. Each pixel is an 8-bit unsigned integer (`uint8`) with values between 0 and 255. It is stored in a 3D NDArray. Its last dimension is the number of channels. Since the data set is a grayscale image, the number of channels is 1. When we encounter color, images, we'll have 3 channels for red, green, and blue. To keep things simple, we will record the shape of the image with the height and width of  $h$  and  $w$  pixels, respectively, as  $h \times w$  or  $(h, w)$ .

```
image.shape, image.dtype
```

```
((28, 28), numpy.float32)
```

The label of each image is represented as a scalar in NumPy. Its type is a 32-bit integer.

```
label, type(label), label.dtype
```

```
(4, numpy.int32, dtype('int32'))
```

We can also access multiple examples at the same time.

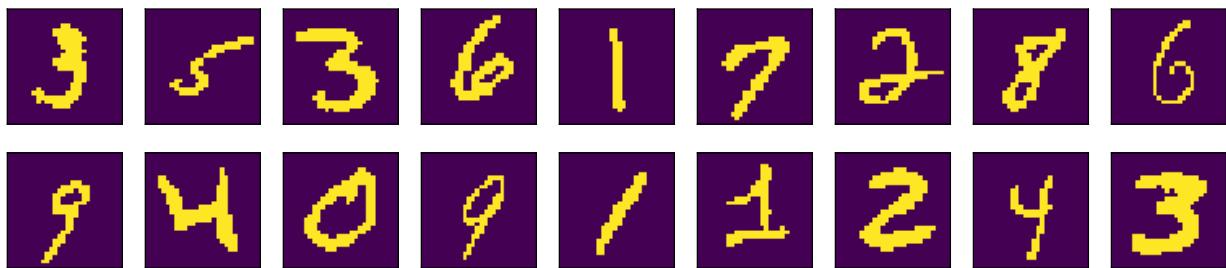
```
images, labels = mnist_train[10:38]
images.shape, labels.shape
```

```
((28, 28, 28), (28,))
```

Now let's create a function to visualize these examples.

```
# Save to the d2l package.
def show_images(imgs, num_rows, num_cols, titles=None, scale=1.5):
    """Plot a list of images."""
    figsize = (num_cols * scale, num_rows * scale)
    _, axes = d2l.plt.subplots(num_rows, num_cols, figsize=figsize)
    axes = axes.flatten()
    for i, (ax, img) in enumerate(zip(axes, imgs)):
        ax.imshow(img.asnumpy())
        ax.axes.get_xaxis().set_visible(False)
        ax.axes.get_yaxis().set_visible(False)
        if titles:
            ax.set_title(titles[i])
    return axes

show_images(images, 2, 9);
```



### 4.5.2 The Probabilistic Model for Classification

In a classification task, we map an example into a category. Here an example is a grayscale  $28 \times 28$  image, and a category is a digit. (Refer to [Section 5.4](#) for a more detailed explanation.) One natural way to express the classification task is via the probabilistic question: what is the most likely label given the features (i.e. image pixels)? Denote by  $\mathbf{x} \in \mathbb{R}^d$  the features of the example and  $y \in \mathbb{R}$  the label. Here features are image pixels, where we can reshape a 2-dimensional image to a vector so that  $d = 28^2 = 784$ , and labels are digits. We will formally define general features and labels in [Section 5.1](#). The  $p(y|\mathbf{x})$  is the probability of the label given the features. If we are able to compute these probabilities, which are  $p(y|\mathbf{x})$  for  $y = 0, \dots, 9$  in our example, then the classifier will output the prediction  $\hat{y}$  given by the expression:

$$\hat{y} = \operatorname{argmax} p(y|\mathbf{x}). \quad (4.5.1)$$

Unfortunately, this requires that we estimate  $p(y|\mathbf{x})$  for every value of  $\mathbf{x} = x_1, \dots, x_d$ . Imagine that each feature could take one of 2 values. For example, the feature  $x_1 = 1$  might signify that the word apple appears in a given document and  $x_1 = 0$  would signify that it does not. If we had 30 such binary features, that would mean that we need to be prepared to classify any of  $2^{30}$  (over 1 billion!) possible values of the input vector  $\mathbf{x}$ .

Moreover, where is the learning? If we need to see every single possible example in order to predict the corresponding label then we're not really learning a pattern but just memorizing the dataset.

### 4.5.3 The Naive Bayes Classifier

Fortunately, by making some assumptions about conditional independence, we can introduce some inductive bias and build a model capable of generalizing from a comparatively modest selection of training examples. To begin, let's use Bayes Theorem, to express the classifier as

$$\hat{y} = \operatorname{argmax}_y p(y|\mathbf{x}) = \operatorname{argmax}_y \frac{p(\mathbf{x}|y)p(y)}{p(\mathbf{x})}. \quad (4.5.2)$$

Note that the denominator is the normalizing term  $p(\mathbf{x})$  which does not depend on the value of the label  $y$ . As a result, we only need to worry about comparing the numerator across different values of  $y$ . Even if calculating the denominator turned out to be intractable, we could get away with ignoring it, so long as we could evaluate the numerator. Fortunately, however, even if we wanted to recover the normalizing constant, we could, since we know that  $\sum_y p(y|\mathbf{x}) = 1$ , hence we can always recover the normalization term.

Now, let's focus on  $p(\mathbf{x}|y)$ . Using the chain rule of probability, we can express the term  $p(\mathbf{x}|y)$  as

$$p(x_1|y) \cdot p(x_2|x_1, y) \cdot \dots \cdot p(x_d|x_1, \dots, x_{d-1}, y) \quad (4.5.3)$$

By itself, this expression doesn't get us any further. We still must estimate roughly  $2^d$  parameters. However, if we assume that *the features are conditionally independent of each other, given the label*, then suddenly we're in much better shape, as this term simplifies to  $\prod_i p(x_i|y)$ , giving us the predictor

$$\hat{y} = \operatorname{argmax}_y \prod_{i=1}^d p(x_i|y)p(y). \quad (4.5.4)$$

If we can estimate  $\prod_i p(x_i = 1|y)$  for every  $i$  and  $y$ , and save its value in  $P_{xy}[i, y]$ , here  $P_{xy}$  is a  $d \times n$  matrix with  $n$  being the number of classes and  $y \in \{1, \dots, n\}$ . In addition, we estimate  $p(y)$  for every  $y$  and save it in  $P_y[y]$ , with  $P_y$  a  $n$ -length vector. Then for any new example  $\mathbf{x}$ , we could compute

$$\hat{y} = \operatorname{argmax}_y \prod_{i=1}^d P_{xy}[x_i, y]P_y[y], \quad (4.5.5)$$

for any  $y$ . So our assumption of conditional independence has taken the complexity of our model from an exponential dependence on the number of features  $O(2^d n)$  to a linear dependence, which is  $O(dn)$ .

### 4.5.4 Training

The problem now is that we don't actually know  $P_{xy}$  and  $P_y$ . So we need to estimate their values given some training data first. This is what is called *training* the model. Estimating  $P_y$  is not too hard. Since we are only dealing with 10 classes, this is pretty easy - simply count the number of occurrences  $n_y$  for each of the digits and divide it by the total amount of data  $n$ . For instance, if digit 8 occurs  $n_8 = 5,800$  times and we have a total of  $n = 60,000$  images, the probability estimate is  $p(y = 8) = 0.0967$ .

```
X, Y = mnist_train[:] # all training examples

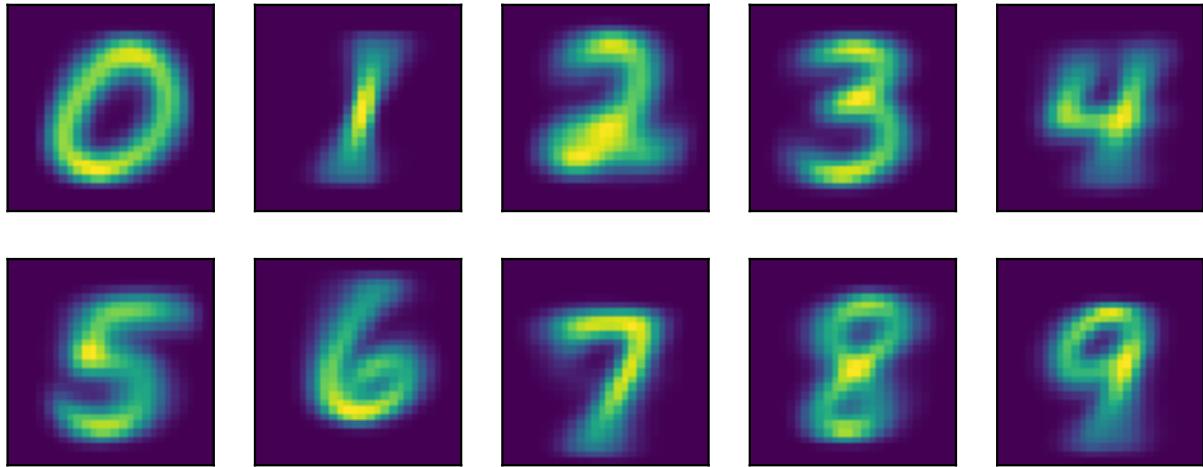
n_y = np.zeros((10))
for y in range(10):
    n_y[y] = (Y==y).sum()
P_y = n_y / n_y.sum()
P_y
```

```
[0.09871667 0.11236667 0.0993      0.10218333 0.09736667 0.09035
 0.09863333 0.10441667 0.09751666 0.09915    ]
<NDArray 10 @cpu(0)>
```

Now on to slightly more difficult things  $P_{xy}$ . Since we picked black and white images,  $p(x_i|y)$  denotes the probability that pixel  $i$  is switched on for class  $y$ . Just like before we can go and count the number of times  $n_{iy}$  such that an event occurs and divide it by the total number of occurrences of  $y$ , i.e.  $n_y$ . But there's something slightly troubling: certain pixels may never be black (e.g. for very well cropped images the corner pixels might always be white). A convenient way for statisticians to deal with this problem is to add pseudo counts to all occurrences. Hence, rather than  $n_{iy}$  we use  $n_{iy} + 1$  and instead of  $n_y$  we use  $n_y + 1$ . This is also called [Laplace Smoothing](#)<sup>51</sup>.

```
n_x = nd.zeros((10, 28, 28))
for y in range(10):
    n_x[y] = nd.array(X.astype(bool)[Y==y].sum(axis=0))
P_xy = (n_x+1) / (n_y+1).reshape((10,1,1))

show_images(P_xy, 2, 5);
```



By visualizing these  $10 \times 28 \times 28$  probabilities (for each pixel for each class) we could get some mean looking digits. ...

Now we can use (4.5.5) to predict a new image. Given  $\mathbf{x}$ , the following functions computes  $p(\mathbf{x}|y)p(y)$  for every  $y$ .

```
def bayes_pred(x):
    x = x.expand_dims(axis=0) # (28, 28) -> (1, 28, 28)
    p_xy = P_xy * x + (1-P_xy)*(1-x)
    p_xy = p_xy.reshape((10,-1)).prod(axis=1) # p(x/y)
    return p_xy * P_y

image, label = mnist_test[0]
bayes_pred(image)
```

<sup>51</sup> [https://en.wikipedia.org/wiki/Additive\\_smoothing](https://en.wikipedia.org/wiki/Additive_smoothing)

```
[0. 0. 0. 0. 0. 0. 0. 0. 0.]  
<NDArray 10 @cpu(0)>
```

This went horribly wrong! To find out why, let's look at the per pixel probabilities. They're typically numbers between 0.001 and 1. We are multiplying 784 of them. At this point it is worth mentioning that we are calculating these numbers on a computer, hence with a fixed range for the exponent. What happens is that we experience *numerical underflow*, i.e. multiplying all the small numbers leads to something even smaller until it is rounded down to zero.

To fix this we use the fact that  $\log ab = \log a + \log b$ , i.e. we switch to summing logarithms. Even if both  $a$  and  $b$  are small numbers, the logarithm values should be in a proper range.

```
a = 0.1  
print('underflow:', a**784)  
print('logarithm is normal:', 784*math.log(a))
```

```
underflow: 0.0  
logarithm is normal: -1805.2267129073316
```

Since the logarithm is an increasing function, so we can rewrite (4.5.5) as

$$\hat{y} = \operatorname{argmax}_y \sum_{i=1}^d \log P_{xy}[x_i, y] + \log P_y[y]. \quad (4.5.6)$$

We can implement the following stable version:

```
log_P_xy = nd.log(P_xy)  
log_P_xy_neg = nd.log(1-P_xy)  
log_P_y = nd.log(P_y)  
  
def bayes_pred_stable(x):  
    x = x.expand_dims(axis=0) # (28, 28) -> (1, 28, 28)  
    p_xy = log_P_xy * x + log_P_xy_neg * (1-x)  
    p_xy = p_xy.reshape((10,-1)).sum(axis=1) # p(x/y)  
    return p_xy + log_P_y  
  
py = bayes_pred_stable(image)
```

```
[-269.00424 -301.73447 -245.21458 -218.8941 -193.46907 -206.10315  
 -292.54315 -114.62834 -220.35619 -163.18881]  
<NDArray 10 @cpu(0)>
```

Check if the prediction is correct.

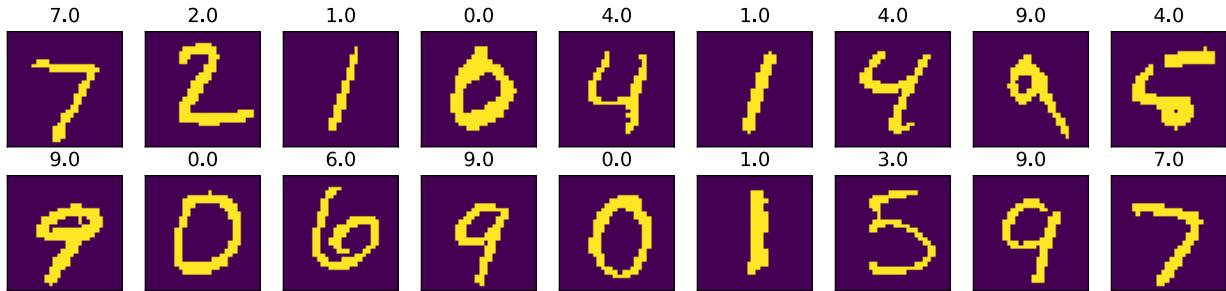
```
py.argmax(axis=0).asscalar() == label
```

```
True
```

Now predict a few validation examples, we can see the Bayes classifier works pretty well except for the 9th 16th digits.

```
def predict(X):
    return [bayes_pred_stable(x).argmax(axis=0).asscalar() for x in X]

X, y = mnist_test[:18]
show_images(X, 2, 9, titles=predict(X));
```



Finally, let's compute the overall accuracy of the classifier.

```
X, y = mnist_test[:]
py = predict(X)
'Validation accuracy', (nd.array(py).asnumpy() == y).sum() / len(y)
```

```
('Validation accuracy', 0.8426)
```

Modern deep networks achieve error rates of less than 0.01. While Naive Bayes classifiers used to be popular in the 80s and 90s, e.g. for spam filtering, their heydays are over. The poor performance is due to the incorrect statistical assumptions that we made in our model: we assumed that each and every pixel are *independently* generated, depending only on the label. This is clearly not how humans write digits, and this wrong assumption led to the downfall of our overly naive (Bayes) classifier. Time to start building Deep Networks.

#### 4.5.5 Summary

- Naive Bayes is an easy to use classifier that uses the assumption  $p(\mathbf{x}|y) = \prod_i p(x_i|y)$ .
- The classifier is easy to train but its estimates can be very wrong.
- To address overly confident and nonsensical estimates, the probabilities  $p(x_i|y)$  are smoothed, e.g. by Laplace smoothing. That is, we add a constant to all counts.
- Naive Bayes classifiers don't exploit any correlations between observations.

#### 4.5.6 Exercises

1. Design a Naive Bayes regression estimator where  $p(x_i|y)$  is a normal distribution.
2. Under which situations does Naive Bayes work?
3. An eyewitness is sure that he could recognize the perpetrator with 90% accuracy, if he were to encounter him again.
  - Is this a useful statement if there are only 5 suspects?
  - Is it still useful if there are 50?

#### 4.5.7 Scan the QR Code to Discuss<sup>52</sup>



## 4.6 Documentation

Due to constraints on the length of this book, we cannot possibly introduce every single MXNet function and class (and you probably would not want us to). The API documentation and additional tutorials and examples provide plenty of documentation beyond the book. In this section we provide you some guidance to exploring the MXNet API.

### 4.6.1 Finding all the functions and classes in the module

In order to know which functions and classes can be called in a module, we invoke the `dir` function. For instance, we can query all properties in the `nd.random` module as follows:

```
from mxnet import nd
print(dir(nd.random))
```

```
['NDArray', '_Null', '__all__', '__builtins__', '__cached__', '__doc__', '__file__', '__loader__',
 '__name__', '__package__', '__spec__', '_internal', '_random_helper',
 '_current_context', 'exponential', 'exponential_like', 'gamma', 'gamma_like',
 'generalized_negative_binomial', 'generalized_negative_binomial_like', 'multinomial',
 'negative_binomial', 'negative_binomial_like', 'normal', 'normal_like', 'numeric_types',
 'poisson', 'poisson_like', 'randint', 'randn', 'shuffle', 'uniform', 'uniform_like']
```

Generally, we can ignore functions that start and end with `__` (special objects in Python) or functions that start with a single `_` (usually internal functions). Based on the remaining function/attribute names, we might hazard a guess that this module offers various methods for generating random numbers, including sampling from the uniform distribution (`uniform`), normal distribution (`normal`), and Poisson distribution (`poisson`).

### 4.6.2 Finding the usage of specific functions and classes

For more specific instructions on how to use a given function or class, we can invoke the `help` function. As an example, let's explore the usage instructions for NDArray's `ones_like` function.

```
help(nd.ones_like)
```

```
Help on function ones_like:
```

```
ones_like(data=None, out=None, name=None, **kwargs)
    Return an array of ones with the same shape and type
```

(continues on next page)

<sup>52</sup> <https://discuss.mxnet.io/t/2320>

(continued from previous page)

```
as the input array.
```

Examples::

```
x = [[ 0.,  0.,  0.],
      [ 0.,  0.,  0.]]

ones_like(x) = [[ 1.,  1.,  1.],
                 [ 1.,  1.,  1.]]
```

Parameters

```
-----  
data : NDArray  
    The input
```

```
out : NDArray, optional  
    The output NDArray to hold the result.
```

Returns

```
-----  
out : NDArray or list of NDArrays  
    The output of this function.
```

From the documentation, we can see that the `ones_like` function creates a new array with the same shape as the supplied NDArray and all elements set to 1. Whenever possible, you should run a quick test to confirm your interpretation:

```
x = nd.array([[0, 0, 0], [2, 2, 2]])
y = x.ones_like()
y
```

```
[[1. 1. 1.]
 [1. 1. 1.]]
<NDArray 2x3 @cpu(0)>
```

In the Jupyter notebook, we can use `?` to display the document in another window. For example, `nd.random.uniform?` will create content that is almost identical to `help(nd.random.uniform)`, displaying it in a new browser window. In addition, if we use two question marks, e.g. `nd.random.uniform??`, the code implementing the function will also be displayed.

### 4.6.3 API Documentation

For further details on the API details check the MXNet website at <http://mxnet.apache.org/>. You can find the details under the appropriate headings (also for programming languages other than Python).

### 4.6.4 Exercise

Look up `ones_like` and `autograd` in the API documentation.

#### 4.6.5 Scan the QR Code to Discuss<sup>53</sup>



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<sup>53</sup> <https://discuss.mxnet.io/t/2322>



## LINEAR NEURAL NETWORKS

Before we get into the details of deep neural networks, we need to cover the basics of neural network training. In this chapter, we will cover the entire training process, including defining simple neural network architectures, handling data, specifying a loss function, and training the model. In order to make things easier to grasp, we begin with the simplest concepts. Fortunately, classic statistical learning techniques such as linear and logistic regression can be cast as *shallow* neural networks. Starting from these classic algorithms, we'll introduce you to the basics, providing the basis for more complex techniques such as softmax regression (introduced at the end of this chapter) and multilayer perceptrons (introduced in the next chapter).

### 5.1 Linear Regression

To start off, we will introduce the problem of regression. This is the task of predicting a *real valued target*  $y$  given a data point  $\mathbf{x}$ . Regression problems are common in practice, arising whenever we want to predict a continuous numerical value. Some examples of regression problems include predicting house prices, stock prices, length of stay (for patients in the hospital), tomorrow's temperature, demand forecasting (for retail sales), and many more. Note that not every prediction problem is a regression problem. In subsequent sections we will discuss classification problems, where our predictions are discrete categories.

#### 5.1.1 Basic Elements of Linear Regression

Linear regression, which dates to Gauss and Legendre, is perhaps the simplest, and by far the most popular approach to solving regression problems. What makes linear regression *linear* is that we assume that the output truly can be expressed as a *linear* combination of the input features.

##### Linear Model

To keep things simple, we will start with running example in which we consider the problem of estimating the price of a house (e.g. in dollars) based on area (e.g. in square feet) and age (e.g. in years). More formally, the assumption of linearity suggests that our model can be expressed in the following form:

$$\text{price} = w_{\text{area}} \cdot \text{area} + w_{\text{age}} \cdot \text{age} + b \quad (5.1.1)$$

In economics papers, it is common for authors to write out linear models in this format with a gigantic equation that spans multiple lines containing terms for every single feature. For the high-dimensional data that we often address in machine learning, writing out the entire model can be tedious. In these cases, we will find it more convenient to use linear algebra notation. In the case of  $d$  variables, we could express our prediction  $\hat{y}$  as follows:

$$\hat{y} = w_1 \cdot x_1 + \dots + w_d \cdot x_d + b \quad (5.1.2)$$

or alternatively, collecting all features into a single vector  $\mathbf{x}$  and all parameters into a vector  $\mathbf{w}$ , we can express our linear model as

$$\hat{y} = \mathbf{w}^T \mathbf{x} + b. \quad (5.1.3)$$

Above, the vector  $\mathbf{x}$  corresponds to a single data point. Commonly, we will want notation to refer to the entire dataset of all input data points. This matrix, often denoted using a capital letter  $X$ , is called the *design matrix* and contains one row for every example, and one column for every feature.

Given a collection of data points  $X$  and a vector containing the corresponding target values  $\mathbf{y}$ , the goal of linear regression is to find the *weight* vector  $w$  and bias term  $b$  (also called an *offset* or *intercept*) that associates each data point  $\mathbf{x}_i$  with an approximation  $\hat{y}_i$  of its corresponding label  $y_i$ .

Expressed in terms of a single data point, this gives us the expression same as (5.1.3).

Finally, for a collection of data points  $\mathbf{X}$ , the predictions  $\hat{\mathbf{y}}$  can be expressed via the matrix-vector product:

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{w} + b. \quad (5.1.4)$$

Even if we believe that the best model to relate  $\mathbf{x}$  and  $y$  is linear, it's unlikely that we'd find data where  $y$  lines up exactly as a linear function of  $\mathbf{x}$ . For example, both the target values  $y$  and the features  $X$  might be subject to some amount of measurement error. Thus even when we believe that the linearity assumption holds, we will typically incorporate a noise term to account for such errors.

Before we can go about solving for the best setting of the parameters  $w$  and  $b$ , we will need two more things: (i) some way to measure the quality of the current model and (ii) some way to manipulate the model to improve its quality.

## Training Data

The first thing that we need is training data. Sticking with our running example, we'll need some collection of examples for which we know both the actual selling price of each house as well as their corresponding area and age. Our goal is to identify model parameters that minimize the error between the predicted price and the real price. In the terminology of machine learning, the data set is called a *training data* or *training set*, a house (often a house and its price) here comprises one *sample*, and its actual selling price is called a *label*. The two factors used to predict the label are called *features* or *covariates*.

Typically, we will use  $n$  to denote the number of samples in our dataset. We index the samples by  $i$ , denoting each input data point as  $x^{(i)} = [x_1^{(i)}, x_2^{(i)}]$  and the corresponding label as  $y^{(i)}$ .

## Loss Function

In model training, we need to measure the error between the predicted value and the real value of the price. Usually, we will choose a non-negative number as the error. The smaller the value, the smaller the error. A common choice is the square function. For given parameters  $\mathbf{w}$  and  $b$ , we can express the error of our prediction on a given a sample as follows:

$$l^{(i)}(\mathbf{w}, b) = \frac{1}{2} (\hat{y}^{(i)} - y^{(i)})^2, \quad (5.1.5)$$

The constant  $1/2$  is just for mathematical convenience, ensuring that after we take the derivative of the loss, the constant coefficient will be 1. The smaller the error, the closer the predicted price is to the actual price, and when the two are equal, the error will be zero.

Since the training dataset is given to us, and thus out of our control, the error is only a function of the model parameters. In machine learning, we call the function that measures the error the *loss function*. The squared error function used here is commonly referred to as *square loss*.

To make things a bit more concrete, consider the example below where we plot a regression problem for a one-dimensional case, e.g. for a model where house prices depend only on area.

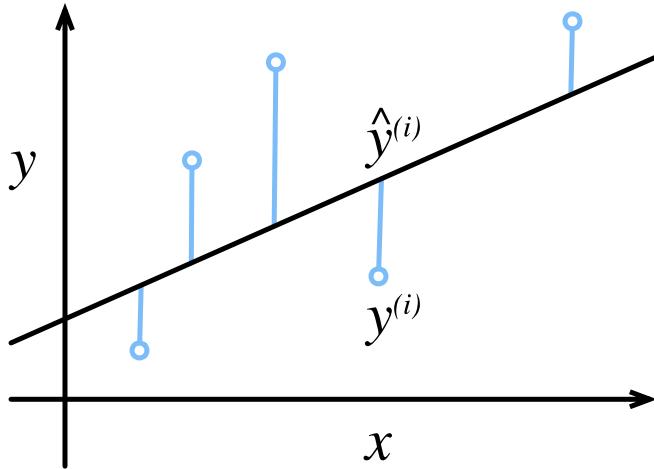


Fig. 5.1.1: Fit data with a linear model.

As you can see, large differences between estimates  $\hat{y}^{(i)}$  and observations  $y^{(i)}$  lead to even larger contributions in terms of the loss, due to the quadratic dependence. To measure the quality of a model on the entire dataset, we can simply average the losses on the training set.

$$L(\mathbf{w}, b) = \frac{1}{n} \sum_{i=1}^n l^{(i)}(\mathbf{w}, b) = \frac{1}{n} \sum_{i=1}^n \frac{1}{2} \left( \mathbf{w}^\top \mathbf{x}^{(i)} + b - y^{(i)} \right)^2. \quad (5.1.6)$$

When training the model, we want to find parameters  $(\mathbf{w}^*, b^*)$  that minimize the average loss across all training samples:

$$\mathbf{w}^*, b^* = \underset{\mathbf{w}, b}{\operatorname{argmin}} L(\mathbf{w}, b). \quad (5.1.7)$$

### Analytic Solution

Linear regression happens to be an unusually simple optimization problem. Unlike nearly every other model that we will encounter in this book, linear regression can be solved easily with a simple formula, yielding a global optimum. To start we can subsume the bias  $b$  into the parameter  $\mathbf{w}$  by appending a column to the design matrix consisting of all 1s. Then our prediction problem is to minimize  $\|\mathbf{y} - \mathbf{X}\mathbf{w}\|$ . Because this expression has a quadratic form it is clearly convex, and so long as the problem is not degenerate (our features are linearly independent), it is strictly convex.

Thus there is just one global critical point on the loss surface corresponding to the global minimum. Taking the derivative of the loss with respect to  $\mathbf{w}$  and setting it equal to 0 gives the analytic solution:

$$\mathbf{w}^* = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} \quad (5.1.8)$$

While simple problems like linear regression may admit analytic solutions, you should not get used to such good fortune. Although analytic solutions allow for nice mathematical analysis, the requirement of an analytic solution confines one to a restrictive set of models that would exclude all of deep learning.

## Gradient descent

Even in cases where we cannot solve the models analytically, and even when the loss surfaces are high-dimensional and nonconvex, it turns out that we can still make progress. Moreover, when those difficult-to-optimize models are sufficiently superior for the task at hand, figuring out how to train them is well worth the trouble.

The key trick behind nearly all of deep learning and that we will repeatedly throughout this book is to reduce the error gradually by iteratively updating the parameters, each step moving the parameters in the direction that incrementally lowers the loss function. This algorithm is called gradient descent. On convex loss surfaces it will eventually converge to a global minimum, and while the same can't be said for nonconvex surfaces, it will at least lead towards a (hopefully good) local minimum.

The most naive application of gradient descent consists of taking the derivative of the true loss, which is an average of the losses computed on every single example in the dataset. In practice, this can be extremely slow. We must pass over the entire dataset before making a single update. Thus, we'll often settle for sampling a random mini-batch of examples every time we need to computer the update, a variant called *stochastic gradient descent*.

In each iteration, we first randomly and uniformly sample a mini-batch  $\mathcal{B}$  consisting of a fixed number of training data examples. We then compute the derivative (gradient) of the average loss on the mini batch with regard to the model parameters. Finally, the product of this result and a predetermined step size  $\eta > 0$  are used to update the parameters in the direction that lowers the loss.

We can express the update mathematically as follows ( $\partial$  denotes the partial derivative):

$$(\mathbf{w}, b) \leftarrow (\mathbf{w}, b) - \frac{\eta}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \partial_{(\mathbf{w}, b)} l^{(i)}(\mathbf{w}, b) \quad (5.1.9)$$

To summarize, steps of the algorithm are the following: (i) we initialize the values of the model parameters, typically at random; (ii) we iterate over the data many times, updating the parameters in each by moving the parameters in the direction of the negative gradient, as calculated on a random minibatch of data.

For quadratic losses and linear functions we can write this out explicitly as follows. Note that  $\mathbf{w}$  and  $\mathbf{x}$  are vectors. Here the more elegant vector notation makes the math much more readable than expressing things in terms of coefficients, say  $w_1, w_2, \dots, w_d$ .

$$\begin{aligned} \mathbf{w} \leftarrow \mathbf{w} - \frac{\eta}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \partial_{\mathbf{w}} l^{(i)}(\mathbf{w}, b) &= w - \frac{\eta}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \mathbf{x}^{(i)} \left( \mathbf{w}^\top \mathbf{x}^{(i)} + b - y^{(i)} \right), \\ b \leftarrow b - \frac{\eta}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \partial_b l^{(i)}(\mathbf{w}, b) &= b - \frac{\eta}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \left( \mathbf{w}^\top \mathbf{x}^{(i)} + b - y^{(i)} \right). \end{aligned} \quad (5.1.10)$$

In the above equation  $|\mathcal{B}|$  represents the number of samples (batch size) in each mini-batch,  $\eta$  is referred to as *learning rate* and takes a positive number. It should be emphasized that the values of the batch size and learning rate are set somewhat manually and are typically not learned through model training. Therefore, they are referred to as *hyper-parameters*. What we usually call *tuning hyper-parameters* refers to the adjustment of these terms. In the worst case this is performed through repeated trial and error until the appropriate hyper-parameters are found. A better approach is to learn these as parts of model training. This is an advanced topic and we do not cover them here for the sake of simplicity.

## Model Prediction

After completing the training process, we record the estimated model parameters, denoted  $\hat{\mathbf{w}}, \hat{b}$  (in general the “hat” symbol denotes estimates). Note that the parameters that we learn via gradient descent are not exactly equal to the true minimizers of the loss on the training set, that's because gradient descent converges slowly to a local minimum but does not achieve it exactly. Moreover if the problem has multiple local minimum, we

may not necessarily achieve the lowest minimum. Fortunately, for deep neural networks, finding parameters that minimize the loss *on training data* is seldom a significant problem. The more formidable task is to find parameters that will achieve low loss on data that we have not seen before, a challenge called *generalization*. We return to these topics throughout the book.

Given the learned linear regression model  $\hat{\mathbf{w}}^\top \mathbf{x} + \hat{b}$ , we can now estimate the price of any house outside the training data set with area (square feet) as  $x_1$  and house age (year) as  $x_2$ . Here, estimation also referred to as ‘model prediction’ or ‘model inference’.

Note that calling this step *inference* is a misnomer, but has become standard jargon in deep learning. In statistics, inference means estimating parameters and outcomes based on other data. This misuse of terminology in deep learning can be a source of confusion when talking to statisticians.

### 5.1.2 From Linear Regression to Deep Networks

So far we only talked about linear functions. While neural networks cover a much richer family of models, we can begin thinking of the linear model as a neural network by expressing it in the language of neural networks. To begin, let’s start by rewriting things in a ‘layer’ notation.

#### Neural Network Diagram

Commonly, deep learning practitioners represent models visually using neural network diagrams. In Fig. 5.1.2, we represent linear regression with a neural network diagram. The diagram shows the connectivity among the inputs and output, but does not depict the weights or biases (which are given implicitly).

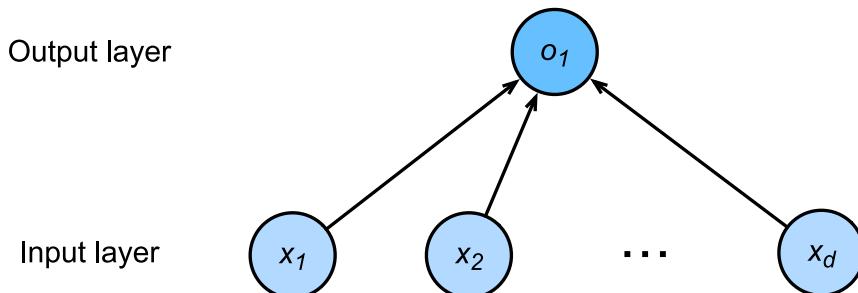


Fig. 5.1.2: Linear regression is a single-layer neural network.

In the above network, the inputs are  $x_1, x_2, \dots, x_d$ . Sometimes the number of inputs are referred to as the feature dimension. For linear regression models, we act upon  $d$  inputs and output 1 value. Because there is just a single computed neuron (node) in the graph, we can think of linear models as neural networks consisting of just a single neuron. Since all inputs are connected to all outputs (in this case it’s just one), this layer can also be regarded as an instance of a *fully-connected layer*, also commonly called a *dense layer*.

#### Biology

Neural networks derive their name from their inspirations in neuroscience. Although linear regression predates computation neuroscience, many of the models we subsequently discuss truly owe to neural inspiration. To understand the neural inspiration for artificial neural networks it is worth while considering the basic structure of a neuron. For the purpose of the analogy it is sufficient to consider the *dendrites* (input terminals), the *nucleus* (CPU), the *axon* (output wire), and the *axon terminals* (output terminals) which connect to other neurons via *synapses*.

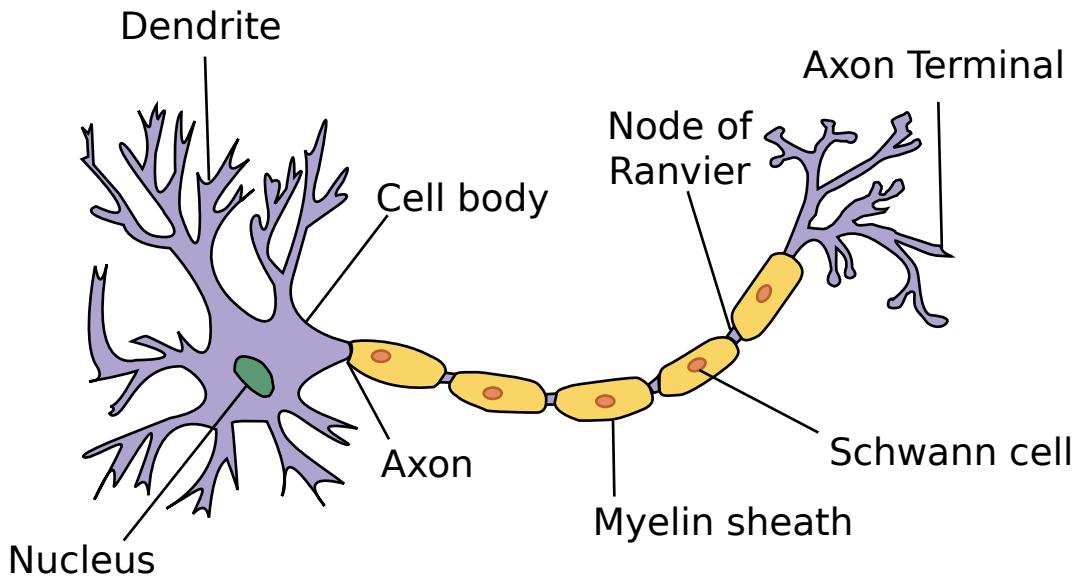


Fig. 5.1.3: The real neuron

Information  $x_i$  arriving from other neurons (or environmental sensors such as the retina) is received in the dendrites. In particular, that information is weighted by *synaptic weights*  $w_i$  which determine how to respond to the inputs (e.g. activation or inhibition via  $x_i w_i$ ). All this is aggregated in the nucleus  $y = \sum_i x_i w_i + b$ , and this information is then sent for further processing in the axon  $y$ , typically after some nonlinear processing via  $\sigma(y)$ . From there it either reaches its destination (e.g. a muscle) or is fed into another neuron via its dendrites.

Brain *structures* vary significantly. Some look (to us) rather arbitrary whereas others have a regular structure. For example, the visual system of many insects is consistent across members of a species. The analysis of such structures has often inspired neuroscientists to propose new architectures, and in some cases, this has been successful. However, much research in artificial neural networks has little to do with any direct inspiration in neuroscience, just as although airplanes are *inspired* by birds, the study of ornithology hasn't been the primary driver of aeronautics innovation in the last century. Equal amounts of inspiration these days comes from mathematics, statistics, and computer science.

### Vectorization for Speed

In model training or prediction, we often use vector calculations and process multiple observations at the same time. To illustrate why this matters, consider two methods of adding vectors. We begin by creating two 100000 dimensional ones first.

```
%matplotlib inline
import d2l
import numpy as np
import math
from mxnet import nd
import time

n = 100000
a = np.ones(n)
b = np.ones(n)
```

Since we will benchmark the running time frequently in this book, let's define a timer to do simply analysis of the running time.

```
# Save to the d2l package.
class Timer(object):
    """Record multiple running times."""
    def __init__(self):
        self.times = []
        self.start()

    def start(self):
        """Start the timer"""
        self.start_time = time.time()

    def stop(self):
        """Stop the timer and record the time in a list"""
        self.times.append(time.time() - self.start_time)
        return self.times[-1]

    def avg(self):
        """Return the average time"""
        return sum(self.times)/len(self.times)

    def sum(self):
        """Return the sum of time"""
        return sum(self.times)

    def cumsum(self):
        """Return the accumulated times"""
        return np.array(self.times).cumsum().tolist()
```

Now we can benchmark the workloads. One way to add vectors is to add them one coordinate at a time using a for loop.

```
timer = Timer()
c = np.zeros(n)
for i in range(n):
    c[i] = a[i] + b[i]
'%.5f sec' % timer.stop()
```

```
'0.04099 sec'
```

Another way to add vectors is to add the vectors directly:

```
timer.start()
d = a + b
'%.5f sec' % timer.stop()
```

```
'0.00055 sec'
```

Obviously, the latter is vastly faster than the former. Vectorizing code is a good way of getting order of magnitude speedups. Likewise, as we saw above, it also greatly simplifies the mathematics and with it, it reduces the potential for errors in the notation.

### 5.1.3 The Normal Distribution and Squared Loss

The following is optional and can be skipped but it will greatly help with understanding some of the design choices in building deep learning models. As we saw above, using the squared loss  $l(y, \hat{y}) = \frac{1}{2}(y - \hat{y})^2$  has many nice properties, such as having a particularly simple derivative  $\partial_{\hat{y}} l(y, \hat{y}) = (\hat{y} - y)$ . That is, the gradient is given by the difference between estimate and observation. You might reasonably point out that linear regression is a classical<sup>54</sup> statistical model. Legendre first developed the method of least squares regression in 1805, which was shortly thereafter rediscovered by Gauss in 1809. To understand this a bit better, recall the normal distribution with mean  $\mu$  and variance  $\sigma^2$ .

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right) \quad (5.1.11)$$

Let's define the function to compute the normal distribution.

```
x = np.arange(-7, 7, 0.01)

def normal(x, mu, sigma):
    p = 1 / math.sqrt(2 * math.pi * sigma**2)
    return p * np.exp(- 0.5 / sigma**2 * (x - mu)**2)
```

For a similar reason to create a `Timer` class, we define a `plot` function to draw multiple lines and set the figure properly, since we will visualize lines frequently later.

```
# Save to the d2l package.
def plot(X, Y=None, xlabel=None, ylabel=None, legend=[], xlim=None,
         ylim=None, xscale='linear', yscale='linear', fmts=None,
         figsize=(3.5, 2.5), axes=None):
    """Plot multiple lines"""
    d2l.set_figsize(figsize)
    axes = axes if axes else d2l.plt.gca()
    if isinstance(X, nd.NDArray): X = X.asnumpy()
    if isinstance(Y, nd.NDArray): Y = Y.asnumpy()
    if not hasattr(X[0], '__len__'): X = [X]
    if Y is None: X, Y = [[]]*len(X), X
    if not hasattr(Y[0], '__len__'): Y = [Y]
    if len(X) != len(Y): X = X * len(Y)
    if not fmts: fmts = ['-'*len(X)]
    axes.cla()
    for x, y, fmt in zip(X, Y, fmts):
        if isinstance(x, nd.NDArray): x = x.asnumpy()
        if isinstance(y, nd.NDArray): y = y.asnumpy()
        if len(x):
            axes.plot(x, y, fmt)
        else:
            axes.plot(y, fmt)
    set_axes(axes, xlabel, ylabel, xlim, ylim, xscale, yscale, legend)

# Save to the d2l package.
def set_axes(axes, xlabel, ylabel, xlim, ylim, xscale, yscale, legend):
    """A utility function to set matplotlib axes"""
    axes.set_xlabel(xlabel)
    axes.set_ylabel(ylabel)
```

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<sup>54</sup> [https://en.wikipedia.org/wiki/Regression\\_analysis#History](https://en.wikipedia.org/wiki/Regression_analysis#History)

(continued from previous page)

```

axes.set_xscale(xscale)
axes.set_yscale(yscale)
axes.set_xlim(xlim)
axes.set_ylim(ylim)
if legend: axes.legend(legend)
axes.grid()

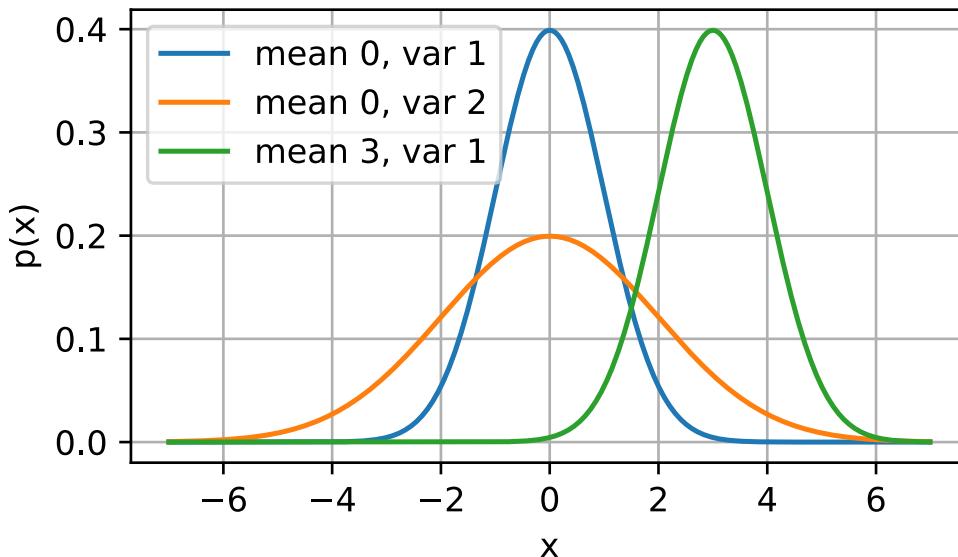
```

Now visualize the normal distributions.

```

# Mean and variance pairs
parameters = [(0,1), (0,2), (3,1)]
plot(x, [normal(x, mu, sigma) for mu, sigma in parameters],
      xlabel='x', ylabel='p(x)', figsize=(4.5, 2.5),
      legend = ['mean %d, var %d' %(mu, sigma) for mu, sigma in parameters])

```



As can be seen in the figure above, changing the mean shifts the function, increasing the variance makes it more spread-out with a lower peak. The key assumption in linear regression with least mean squares loss is that the observations actually arise from noisy observations, where noise is added to the data, e.g. as part of the observations process.

$$y = \mathbf{w}^\top \mathbf{x} + b + \epsilon \text{ where } \epsilon \sim \mathcal{N}(0, \sigma^2) \quad (5.1.12)$$

This allows us to write out the *likelihood* of seeing a particular  $y$  for a given  $\mathbf{x}$  via

$$p(y|\mathbf{x}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(y - \mathbf{w}^\top \mathbf{x} - b)^2\right) \quad (5.1.13)$$

A good way of finding the most likely values of  $b$  and  $\mathbf{w}$  is to maximize the *likelihood* of the entire dataset

$$p(Y|X) = \prod_{i=1}^n p(y^{(i)}|\mathbf{x}^{(i)}) \quad (5.1.14)$$

The notion of maximizing the likelihood of the data subject to the parameters is well known as the *Maximum Likelihood Principle* and its estimators are usually called *Maximum Likelihood Estimators* (MLE).

Unfortunately, maximizing the product of many exponential functions is pretty awkward, both in terms of implementation and in terms of writing it out on paper. Instead, a much better way is to minimize the *Negative Log-Likelihood*  $-\log p(\mathbf{y}|\mathbf{X})$ . In the above case this works out to be

$$-\log p(\mathbf{y}|\mathbf{X}) = \sum_{i=1}^n \frac{1}{2} \log(2\pi\sigma^2) + \frac{1}{2\sigma^2} \left( y^{(i)} - \mathbf{w}^\top \mathbf{x}^{(i)} - b \right)^2 \quad (5.1.15)$$

A closer inspection reveals that for the purpose of minimizing  $-\log p(\mathbf{y}|\mathbf{X})$  we can skip the first term since it doesn't depend on  $\mathbf{w}, b$  or even the data. The second term is identical to the objective we initially introduced, but for the multiplicative constant  $\frac{1}{\sigma^2}$ . Again, this can be skipped if we just want to get the most likely solution. It follows that maximum likelihood in a linear model with additive Gaussian noise is equivalent to linear regression with squared loss.

### 5.1.4 Summary

- Key ingredients in a machine learning model are training data, a loss function, an optimization algorithm, and quite obviously, the model itself.
- Vectorizing makes everything better (mostly math) and faster (mostly code).
- Minimizing an objective function and performing maximum likelihood can mean the same thing.
- Linear models are neural networks, too.

### 5.1.5 Exercises

1. Assume that we have some data  $x_1, \dots, x_n \in \mathbb{R}$ . Our goal is to find a constant  $b$  such that  $\sum_i (x_i - b)^2$  is minimized.
  - Find the optimal closed form solution.
  - What does this mean in terms of the Normal distribution?
2. Assume that we want to solve the optimization problem for linear regression with quadratic loss explicitly in closed form. To keep things simple, you can omit the bias  $b$  from the problem.
  - Rewrite the problem in matrix and vector notation (hint - treat all the data as a single matrix).
  - Compute the gradient of the optimization problem with respect to  $w$ .
  - Find the closed form solution by solving a matrix equation.
  - When might this be better than using stochastic gradient descent (i.e. the incremental optimization approach that we discussed above)? When will this break (hint - what happens for high-dimensional  $x$ , what if many observations are very similar)?
3. Assume that the noise model governing the additive noise  $\epsilon$  is the exponential distribution. That is,  $p(\epsilon) = \frac{1}{2} \exp(-|\epsilon|)$ .
  - Write out the negative log-likelihood of the data under the model  $-\log p(Y|X)$ .
  - Can you find a closed form solution?
  - Suggest a stochastic gradient descent algorithm to solve this problem. What could possibly go wrong (hint - what happens near the stationary point as we keep on updating the parameters). Can you fix this?

### 5.1.6 Scan the QR Code to Discuss<sup>55</sup>



## 5.2 Linear Regression Implementation from Scratch

Now that you have some background on the *ideas* behind linear regression, we are ready to step through a hands-on implementation. In this section, and similar ones that follow, we are going to implement all parts of linear regression: the data pipeline, the model, the loss function, and the gradient descent optimizer, from scratch. Not surprisingly, today's deep learning frameworks can automate nearly all of this work, but if you never learn to implement things from scratch, then you may never truly understand how the model works. Moreover, when it comes time to customize models, defining our own layers, loss functions, etc., knowing how things work under the hood will come in handy. Thus, we start off describing how to implement linear regression relying only on the primitives in the NDArray and autograd packages. In the section immediately following, we will present the compact implementation, using all of Gluon's bells and whistles, but this is where we dive into the details.

To start off, we import the packages required to run this section's experiments.

```
%matplotlib inline
import d2l
from mxnet import autograd, nd
import random
```

### 5.2.1 Generating Data Sets

For this demonstration, we will construct a simple artificial dataset so that we can easily visualize the data and compare the true pattern to the learned parameters. We will set the number of examples in our training set to be 1000 and the number of features (or covariates) to 2. Thus our synthetic dataset will be an object  $\mathbf{X} \in \mathbb{R}^{1000 \times 2}$ . In this example, we will synthesize our data by sampling each data point  $\mathbf{x}_i$  from a Gaussian distribution.

Moreover, to make sure that our algorithm works, we will assume that the linearity assumption holds with true underlying parameters  $\mathbf{w} = [2, -3.4]^\top$  and  $b = 4.2$ . Thus our synthetic labels will be given according to the following linear model which includes a noise term  $\epsilon$  to account for measurement errors on the features and labels:

$$\mathbf{y} = \mathbf{X}\mathbf{w} + b + \epsilon \quad (5.2.1)$$

Following standard assumptions, we choose a noise term  $\epsilon$  that obeys a normal distribution with mean of 0, and in this example, we'll set its standard deviation to 0.01. The following code generates our synthetic dataset:

---

<sup>55</sup> <https://discuss.mxnet.io/t/2331>

```
# Save to the d2l package.
def synthetic_data(w, b, num_examples):
    """generate y = X w + b + noise"""
    X = nd.random.normal(scale=1, shape=(num_examples, len(w)))
    y = nd.dot(X, w) + b
    y += nd.random.normal(scale=0.01, shape=y.shape)
    return X, y

true_w = nd.array([2, -3.4])
true_b = 4.2
features, labels = synthetic_data(true_w, true_b, 1000)
```

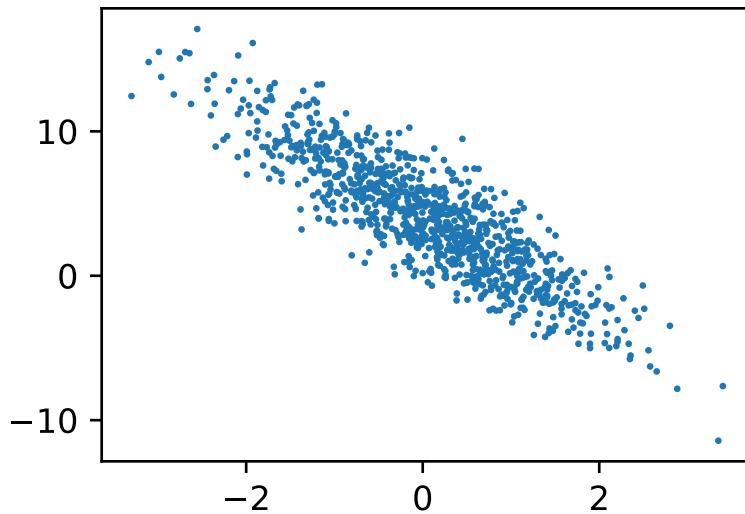
Note that each row in `features` consists of a 2-dimensional data point and that each row in `labels` consists of a 1-dimensional target value (a scalar).

```
features[0], labels[0]
```

```
(  
[2.2122064 0.7740038]  
<NDArray 2 @cpu(0)>,  
[6.000587]  
<NDArray 1 @cpu(0)>)
```

By generating a scatter plot using the second `features[:, 1]` and `labels`, we can clearly observe the linear correlation between the two.

```
d2l.set_figsize((3.5, 2.5))
d2l.plt.scatter(features[:, 1].asnumpy(), labels.asnumpy(), 1);
```



## 5.2.2 Reading Data

Recall that training models, consists of making multiple passes over the dataset, grabbing one mini-batch of examples at a time and using them to update our model. Since this process is so fundamental to training machine learning algorithms, we need a utility for shuffling the data and accessing in mini-batches.

In the following code, we define a `data_iter` function to demonstrate one possible implementation of this functionality. The function takes a batch size, a design matrix containing the features, and a vector of labels, yielding minibatches of size `batch_size`, each consisting of a tuple of features and labels.

```
def data_iter(batch_size, features, labels):
    num_examples = len(features)
    indices = list(range(num_examples))
    # The examples are read at random, in no particular order
    random.shuffle(indices)
    for i in range(0, num_examples, batch_size):
        j = nd.array(indices[i: min(i + batch_size, num_examples)])
        yield features.take(j), labels.take(j)
        # The "take" function will then return the corresponding element
        # based on the indices
```

In general, note that we want to use reasonably sized minibatches to take advantage of the GPU hardware, which excels at parallelizing operations. Because each example can be fed through our models in parallel and the gradient of the loss function for each example can also be taken in parallel, GPUs allow us to process hundreds of examples in scarcely more time than it might take to process just a single example.

To build some intuition, let's read and print the first small batch of data examples. The shape of the features in each mini-batch tells us both the mini-batch size and the number of input features. Likewise, our mini-batch of labels will have a shape given by `batch_size`.

```
batch_size = 10

for X, y in data_iter(batch_size, features, labels):
    print(X, y)
    break
```

```
[[[-0.99406207  0.24402148]
 [ 1.5865177   0.6106281 ]
 [-1.977209   -0.9998924 ]
 [ 0.23976259  1.4648197 ]
 [ 3.3960576   0.44973052]
 [-1.3360355   1.0035783 ]
 [-0.81052285 -1.1052948 ]
 [ 0.18006966 -2.0615053 ]
 [-1.771029   -0.45138445]
 [ 1.0955427   0.7685205 ]]
<NDArray 10x2 @cpu(0)>
[ 1.4004962  5.3046117  3.6282308 -0.3107588  9.479614  -1.8906523
 6.322081  11.573206  2.1933134  3.7752948]
<NDArray 10 @cpu(0)>
```

It should be no surprise that as we run the iterator, we will obtain distinct minibatches each time until all the data has been exhausted (try this). While the iterator implemented above is good for didactic purposes, it is inefficient in ways that might get us in trouble on real problems. For example, it requires that we load all data in memory and that we perform a lot of random memory access. The built-in iterators implemented in Apache MXNet are considerably efficient and they can deal both with data stored on file and data fed via a data stream.

### 5.2.3 Initialize Model Parameters

Before we can begin optimizing our model's parameters by gradient descent, we need to have some parameters in the first place. In the following code, we initialize weights by sampling random numbers from a normal distribution with mean 0 and a standard deviation of 0.01, setting the bias  $b$  to 0.

```
w = nd.random.normal(scale=0.01, shape=(2, 1))
b = nd.zeros(shape=(1,))
```

Now that we have initialized our parameters, our next task is to update them until they fit our data sufficiently well. Each update will require taking the gradient (a multi-dimensional derivative) of our loss function with respect to the parameters. Given this gradient, we will update each parameter in the direction that reduces the loss.

Since nobody wants to compute gradients explicitly (this is tedious and error prone), we use automatic differentiation to compute the gradient. See [Section 4.3](#) for more details. Recall from the autograd chapter that in order for `autograd` to know that it should store a gradient for our parameters, we need to invoke the `attach_grad` function, allocating memory to store the gradients that we plan to take.

```
w.attach_grad()
b.attach_grad()
```

### 5.2.4 Define the Model

Next, we must define our model, relating its inputs and parameters to its outputs. Recall that to calculate the output of the linear model, we simply take the matrix-vector dot product of the examples  $\mathbf{X}$  and the models weights  $w$ , and add the offset  $b$  to each example. Note that below `nd.dot(X, w)` is a vector and `b` is a scalar. Recall that when we add a vector and a scalar, the scalar is added to each component of the vector.

```
# Save to the d2l package.
def linreg(X, w, b):
    return nd.dot(X, w) + b
```

### 5.2.5 Define the Loss Function

Since updating our model requires taking the gradient of our loss function, we ought to define the loss function first. Here we will use the squared loss function as described in the previous section. In the implementation, we need to transform the true value  $y$  into the predicted value's shape  $y_{\text{hat}}$ . The result returned by the following function will also be the same as the  $y_{\text{hat}}$  shape.

```
# Save to the d2l package.
def squared_loss(y_hat, y):
    return (y_hat - y.reshape(y_hat.shape)) ** 2 / 2
```

### 5.2.6 Define the Optimization Algorithm

As we discussed in the previous section, linear regression has a closed-form solution. However, this isn't a book about linear regression, its a book about deep learning. Since none of the other models that this book introduces can be solved analytically, we will take this opportunity to introduce your first working example of stochastic gradient descent (SGD).

At each step, using one batch randomly drawn from our dataset, we'll estimate the gradient of the loss with respect to our parameters. Then, we'll update our parameters a small amount in the direction that reduces the loss. Assuming that the gradient has already been calculated, each parameter (`param`) already has its gradient stored in `param.grad`. The following code applies the SGD update, given a set of parameters, a learning rate, and a batch size. The size of the update step is determined by the learning rate `lr`. Because our loss is calculated as a sum over the batch of examples, we normalize our step size by the batch size (`batch_size`), so that the magnitude of a typical step size doesn't depend heavily on our choice of the batch size.

```
# Save to the d2l package.
def sgd(params, lr, batch_size):
    for param in params:
        param[:] = param - lr * param.grad / batch_size
```

### 5.2.7 Training

Now that we have all of the parts in place, we are ready to implement the main training loop. It is crucial that you understand this code because you will see training loops that are nearly identical to this one over and over again throughout your career in deep learning.

In each iteration, we will grab minibatches of models, first passing them through our model to obtain a set of predictions. After calculating the loss, we will call the `backward` function to backpropagate through the network, storing the gradients with respect to each parameter in its corresponding `.grad` attribute. Finally, we will call the optimization algorithm `sgd` to update the model parameters. Since we previously set the batch size `batch_size` to 10, the loss shape 1 for each small batch is (10, 1).

In summary, we'll execute the following loop:

- Initialize parameters  $(\mathbf{w}, b)$
- Repeat until done
  - Compute gradient  $\mathbf{g} \leftarrow \partial_{(\mathbf{w}, b)} \frac{1}{B} \sum_{i \in \mathcal{B}} l(\mathbf{x}^i, y^i, \mathbf{w}, b)$
  - Update parameters  $(\mathbf{w}, b) \leftarrow (\mathbf{w}, b) - \eta \mathbf{g}$

In the code below, `l` is a vector of the losses for each example in the minibatch. Because `l` is not a scalar variable, running `l.backward()` adds together the elements in `l` to obtain the new variable and then calculates the gradient.

In each epoch (a pass through the data), we will iterate through the entire dataset (using the `data_iter` function) once passing through every examples in the training dataset (assuming the number of examples is divisible by the batch size). The number of epochs `num_epochs` and the learning rate `lr` are both hyper-parameters, which we set here to 3 and 0.03, respectively. Unfortunately, setting hyper-parameters is tricky and requires some adjustment by trial and error. We elide these details for now but revise them later in Section 12.

```
lr = 0.03  # Learning rate
num_epochs = 3  # Number of iterations
net = linreg  # Our fancy linear model
loss = squared_loss  # 0.5 (y-y')^2

for epoch in range(num_epochs):
    # Assuming the number of examples can be divided by the batch size, all
    # the examples in the training data set are used once in one epoch
    # iteration. The features and tags of mini-batch examples are given by X
```

(continues on next page)

(continued from previous page)

```
# and y respectively
for X, y in data_iter(batch_size, features, labels):
    with autograd.record():
        l = loss(net(X, w, b), y) # Minibatch loss in X and y
        l.backward() # Compute gradient on l with respect to [w,b]
        sgd([w, b], lr, batch_size) # Update parameters using their gradient
train_l = loss(net(features, w, b), labels)
print('epoch %d, loss %f' % (epoch + 1, train_l.mean().asnumpy()))
```

```
epoch 1, loss 0.040436
epoch 2, loss 0.000157
epoch 3, loss 0.000050
```

In this case, because we used synthetic data (that we synthesized ourselves!), we know precisely what the true parameters are. Thus, we can evaluate our success in training by comparing the true parameters with those that we learned through our training loop. Indeed they turn out to be very close to each other.

```
print('Error in estimating w', true_w - w.reshape(true_w.shape))
print('Error in estimating b', true_b - b)
```

```
Error in estimating w
[ 0.00015604 -0.00034165]
<NDArray 2 @cpu(0)>
Error in estimating b
[0.00042248]
<NDArray 1 @cpu(0)>
```

Note that we should not take it for granted that we are able to recover the parameters accurately. This only happens for a special category problems: strongly convex optimization problems with ‘enough’ data to ensure that the noisy samples allow us to recover the underlying dependency. In most cases this is *not* the case. In fact, the parameters of a deep network are rarely the same (or even close) between two different runs, unless all conditions are identical, including the order in which the data is traversed. However, in machine learning we are typically less concerned with recovering true underlying parameters, and more concerned with parameters that lead to accurate prediction. Fortunately, even on difficult optimization problems, that stochastic gradient descent can often lead to remarkably good solutions, due in part to the fact that for the models we will be working with, there exist many sets of parameters that work well.

### 5.2.8 Summary

We saw how a deep network can be implemented and optimized from scratch, using just NDArray and autograd, without any need for defining layers, fancy optimizers, etc. This only scratches the surface of what is possible. In the following sections, we will describe additional models based on the concepts that we have just introduced and learn how to implement them more concisely.

### 5.2.9 Exercises

1. What would happen if we were to initialize the weights  $w = 0$ . Would the algorithm still work?
2. Assume that you’re Georg Simon Ohm<sup>56</sup> trying to come up with a model between voltage and current. Can you use autograd to learn the parameters of your model.

<sup>56</sup> [https://en.wikipedia.org/wiki/Georg\\_Ohm](https://en.wikipedia.org/wiki/Georg_Ohm)

3. Can you use Planck's Law<sup>57</sup> to determine the temperature of an object using spectral energy density.
4. What are the problems you might encounter if you wanted to extend `autograd` to second derivatives? How would you fix them?
5. Why is the `reshape` function needed in the `squared_loss` function?
6. Experiment using different learning rates to find out how fast the loss function value drops.
7. If the number of examples cannot be divided by the batch size, what happens to the `data_iter` function's behavior?

### 5.2.10 Scan the QR Code to Discuss<sup>58</sup>



## 5.3 Concise Implementation of Linear Regression

The surge of deep learning has inspired the development of a variety of mature software frameworks, that automate much of the repetitive work of implementing deep learning models. In the previous section we relied only on `NDarray` for data storage and linear algebra and the auto-differentiation capabilities in the `autograd` package. In practice, because many of the more abstract operations, e.g. data iterators, loss functions, model architectures, and optimizers, are so common, deep learning libraries will give us library functions for these as well.

We have used Gluon to load the MNIST dataset in Section 4.5. In this section, we will learn how we can implement the linear regression model in Section 5.2 much more concisely with Gluon.

### 5.3.1 Generating Data Sets

To start, we will generate the same data set as that used in the previous section.

```
import d2l
from mxnet import autograd, nd, gluon

true_w = nd.array([2, -3.4])
true_b = 4.2
features, labels = d2l.synthetic_data(true_w, true_b, 1000)
```

### 5.3.2 Reading Data

Rather than rolling our own iterator, we can call upon Gluon's `data` module to read data.

<sup>57</sup> [https://en.wikipedia.org/wiki/Planck%27s\\_law](https://en.wikipedia.org/wiki/Planck%27s_law)

<sup>58</sup> <https://discuss.mxnet.io/t/2332>

The first step will be to instantiate an `ArrayDataset`, which takes in one or more NDArrays as arguments. Here, we pass in `features` and `labels` as arguments. Next, we will use the `ArrayDataset` to instantiate a `DataLoader`, which also requires that we specify a `batch_size` and specify a Boolean value `shuffle` indicating whether or not we want the `DataLoader` to shuffle the data on each epoch (pass through the dataset).

```
# Save to the d2l package.
def load_array(data_arrays, batch_size, is_train=True):
    """Construct a Gluon data loader"""
    dataset = gluon.data.ArrayDataset(*data_arrays)
    return gluon.data.DataLoader(dataset, batch_size, shuffle=is_train)

batch_size = 10
data_iter = load_array((features, labels), batch_size)
```

Now we can use `data_iter` in much the same way as we called the `data_iter` function in the previous section. To verify that it's working, we can read and print the first mini-batch of instances.

```
for X, y in data_iter:
    print(X, y)
    break
```

```
[[ -0.3990028 -0.57255214]
 [-1.986459   1.0147698 ]
 [-0.26519665  1.5181851 ]
 [ 0.5952477 -2.1951923 ]
 [-1.436299 -1.2416507 ]
 [-0.9098478 -0.14092611]
 [ 0.8806273  1.9885163 ]
 [ 0.05136351 -1.8751514 ]
 [-1.771029 -0.45138445]
 [-0.41733953  0.5984538 ]]
<NDArray 10x2 @cpu(0)>
[ 5.3430595 -3.2290342 -1.4937832  12.849786   5.559958   2.869347
 -0.79267937 10.687464     2.1933134   1.3308488 ]
<NDArray 10 @cpu(0)>
```

### 5.3.3 Define the Model

When we implemented linear regression from scratch in the previous section, we had to define the model parameters and explicitly write out the calculation to produce output using basic linear algebra operations. You should know how to do this. But once your models get more complex, even qualitatively simple changes to the model might result in many low-level changes.

For standard operations, we can use Gluon's predefined layers, which allow us to focus especially on the layers used to construct the model rather than having to focus on the implementation.

To define a linear model, we first import the `nn` module, which defines a large number of neural network layers (note that "nn" is an abbreviation for neural networks). We will first define a model variable `net`, which is a `Sequential` instance. In Gluon, a `Sequential` instance can be regarded as a container that concatenates the various layers in sequence. When input data is given, each layer in the container will be calculated in order, and the output of one layer will be the input of the next layer. In this example, since our model consists of only one layer, we do not really need `Sequential`. But since nearly all of our future models will involve multiple layers, let's get into the habit early.

```
from mxnet.gluon import nn
net = nn.Sequential()
```

Recall the architecture of a single layer network. The layer is fully connected since it connects all inputs with all outputs by means of a matrix-vector multiplication. In Gluon, the fully-connected layer is defined in the `Dense` class. Since we only want to generate a single scalar output, we set that number to 1.

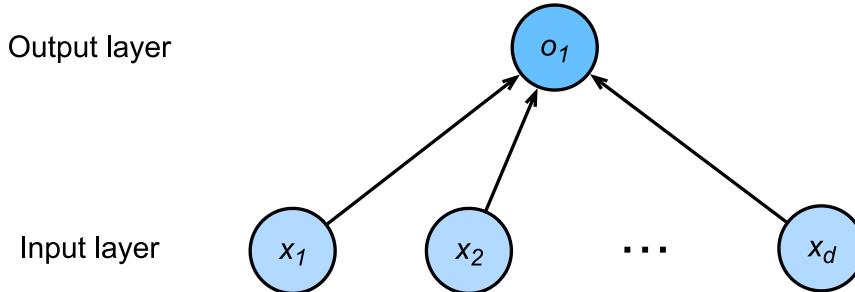


Fig. 5.3.1: Linear regression is a single-layer neural network.

```
net.add(nn.Dense(1))
```

It is worth noting that, for convenience, Gluon does not require us to specify the input shape for each layer. So here, we don't need to tell Gluon how many inputs go into this linear layer. When we first try to pass data through our model, e.g., when we execute `net(X)` later, Gluon will automatically infer the number of inputs to each layer. We will describe how this works in more detail in the chapter “Deep Learning Computation”.

### 5.3.4 Initialize Model Parameters

Before using `net`, we need to initialize the model parameters, such as the weights and biases in the linear regression model. We will import the `initializer` module from MXNet. This module provides various methods for model parameter initialization. Gluon makes `init` available as a shortcut (abbreviation) to access the `initializer` package. By calling `init.Normal(sigma=0.01)`, we specify that each *weight* parameter should be randomly sampled from a normal distribution with mean 0 and standard deviation 0.01. The *bias* parameter will be initialized to zero by default. Both weight and bias will be attached with gradients.

```
from mxnet import init
net.initialize(init.Normal(sigma=0.01))
```

The code above looks straightforward but in reality something quite strange is happening here. We are initializing parameters for a network even though we haven't yet told Gluon how many dimensions the input will have. It might be 2 as in our example or it might be 2,000, so we couldn't just preallocate enough space to make it work.

Gluon let's us get away with this because behind the scenes, the initialization is deferred until the first time that we attempt to pass data through our network. Just be careful to remember that since the parameters have not been initialized yet we cannot yet manipulate them in any way.

### 5.3.5 Define the Loss Function

In Gluon, the `loss` module defines various loss functions. We will replace the imported module `loss` with the pseudonym `gloss`, and directly use its implementation of squared loss (`L2Loss`).

```
from mxnet.gluon import loss as gloss
loss = gloss.L2Loss() # The squared loss is also known as the L2 norm loss
```

### 5.3.6 Define the Optimization Algorithm

Not surprisingly, we aren't the first people to implement mini-batch stochastic gradient descent, and thus Gluon supports SGD alongside a number of variations on this algorithm through its `Trainer` class. When we instantiate the `Trainer`, we'll specify the parameters to optimize over (obtainable from our net via `net.collect_params()`), the optimization algorithm we wish to use (`sgd`), and a dictionary of hyper-parameters required by our optimization algorithm. SGD just requires that we set the value `learning_rate`, (here we set it to 0.03).

```
from mxnet import gluon
trainer = gluon.Trainer(net.collect_params(), 'sgd', {'learning_rate': 0.03})
```

### 5.3.7 Training

You might have noticed that expressing our model through Gluon requires comparatively few lines of code. We didn't have to individually allocate parameters, define our loss function, or implement stochastic gradient descent. Once we start working with much more complex models, the benefits of relying on Gluon's abstractions will grow considerably. But once we have all the basic pieces in place, the training loop itself is strikingly similar to what we did when implementing everything from scratch.

To refresh your memory: for some number of epochs, we'll make a complete pass over the dataset (`train_data`), grabbing one mini-batch of inputs and corresponding ground-truth labels at a time. For each batch, we'll go through the following ritual:

- Generate predictions by calling `net(X)` and calculate the loss `l` (the forward pass).
- Calculate gradients by calling `l.backward()` (the backward pass).
- Update the model parameters by invoking our SGD optimizer (note that `trainer` already knows which parameters to optimize over, so we just need to pass in the batch size).

For good measure, we compute the loss after each epoch and print it to monitor progress.

```
num_epochs = 3
for epoch in range(1, num_epochs + 1):
    for X, y in data_iter:
        with autograd.record():
            l = loss(net(X), y)
        l.backward()
        trainer.step(batch_size)
    l = loss(net(features), labels)
    print('epoch %d, loss: %f' % (epoch, l.mean().asnumpy()))
```

```
epoch 1, loss: 0.040633
epoch 2, loss: 0.000156
epoch 3, loss: 0.000050
```

The model parameters we have learned and the actual model parameters are compared as below. We get the layer we need from the `net` and access its weight (`weight`) and bias (`bias`). The parameters we have learned and the actual parameters are very close.

```
w = net[0].weight.data()
print('Error in estimating w', true_w.reshape(w.shape) - w)
b = net[0].bias.data()
print('Error in estimating b', true_b - b)
```

```
Error in estimating w
[[9.405613e-05 7.867813e-05]]
<NDArray 1x2 @cpu(0)>
Error in estimating b
[0.00016642]
<NDArray 1 @cpu(0)>
```

### 5.3.8 Summary

- Using Gluon, we can implement the model more succinctly.
- In Gluon, the module `data` provides tools for data processing, the module `nn` defines a large number of neural network layers, and the module `loss` defines various loss functions.
- MXNet's module `initializer` provides various methods for model parameter initialization.
- Dimensionality and storage are automatically inferred (but caution if you want to access parameters before they've been initialized).

### 5.3.9 Exercises

1. If we replace `l = loss(output, y)` with `l = loss(output, y).mean()`, we need to change `trainer.step(batch_size)` to `trainer.step(1)` accordingly. Why?
2. Review the MXNet documentation to see what loss functions and initialization methods are provided in the modules `gluon.loss` and `init`. Replace the loss by Huber's loss.
3. How do you access the gradient of `dense.weight`?

### 5.3.10 Scan the QR Code to Discuss<sup>59</sup>



## 5.4 Softmax Regression

In Section 5.1 we introduced linear regression, and worked through building everything from scratch in Section 5.2 and using Gluon in Section 5.3 to automate the most repetitive work.

<sup>59</sup> <https://discuss.mxnet.io/t/2333>

Regression is the hammer we reach for when we want to answer *how much?* or *how many?* questions. If you want to predict the number of dollars (the *price*) at which a house will be sold, or the number of wins a baseball team might have, or the number of days that a patient will remain hospitalized before being discharged, then you're probably looking for a regression model.

In practice, we're more often interested in classification: asking not *how much* but *which one*.

- Does this email belong in the spam folder or the inbox?
- Is this customer more likely *to sign up* or *not to sign up* for a subscription service?
- Does this image depict a donkey, a dog, a cat, or a rooster?
- Which movie is user most likely to watch next?

Colloquially, we use the word *classification* to describe two subtly different problems: (i) those where we are interested only in *hard assignments* of examples to categories, and (ii) those where we wish to make *soft assignments*, i.e., to assess the *probability* that each category applies. One reason why the distinction between these tasks gets blurred is because most often, even when we only care about hard assignments, we still use models that make soft assignments.

### 5.4.1 Classification Problems

To get our feet wet, let's start off with a somewhat contrived image classification problem. Here, each input will be a grayscale 2-by-2 image. We can represent each pixel location as a single scalar, representing each image with four features  $x_1, x_2, x_3, x_4$ . Further, let's assume that each image belongs to one among the categories "cat", "chicken" and "dog".

First, we have to choose how to represent the labels. We have two obvious choices. Perhaps the most natural impulse would be to choose  $y \in \{1, 2, 3\}$ , where the integers represent {dog, cat, chicken} respectively. This is a great way of *storing* such information on a computer. If the categories had some natural ordering among them, say if we were trying to predict {baby, child, adolescent, adult}, then it might even make sense to cast this problem as a regression and keep the labels in this format.

But general classification problems do not come with natural orderings among the classes. To deal with problems like this, statisticians invented an alternative way to represent categorical data: the one hot encoding. Here we have a vector with one component for every possible category. For a given instance, we set the component corresponding to *its category* to 1, and set all other components to 0.

$$y \in \{(1, 0, 0), (0, 1, 0), (0, 0, 1)\} \quad (5.4.1)$$

In our case,  $y$  would be a three-dimensional vector, with  $(1, 0, 0)$  corresponding to "cat",  $(0, 1, 0)$  to "chicken" and  $(0, 0, 1)$  to "dog". It is often called the *one-hot encoding*.

#### Network Architecture

In order to estimate multiple classes, we need a model with multiple outputs, one per category. This is one of the main differences between classification and regression models. To address classification with linear models, we will need as many linear functions as we have outputs. Each output will correspond to its own linear function. In our case, since we have 4 features and 3 possible output categories, we will need 12 scalars to represent the weights, ( $w$  with subscripts) and 3 scalars to represent the biases ( $b$  with subscripts). We compute these three outputs,  $o_1, o_2$ , and  $o_3$ , for each input:

$$\begin{aligned} o_1 &= x_1 w_{11} + x_2 w_{12} + x_3 w_{13} + x_4 w_{14} + b_1, \\ o_2 &= x_1 w_{21} + x_2 w_{22} + x_3 w_{23} + x_4 w_{24} + b_2, \\ o_3 &= x_1 w_{31} + x_2 w_{32} + x_3 w_{33} + x_4 w_{34} + b_3. \end{aligned} \quad (5.4.2)$$

We can depict this calculation with the neural network diagram below. Just as in linear regression, softmax regression is also a single-layer neural network. And since the calculation of each output,  $o_1, o_2$ , and  $o_3$ , depends on all inputs,  $x_1, x_2, x_3$ , and  $x_4$ , the output layer of softmax regression can also be described as fully connected layer.

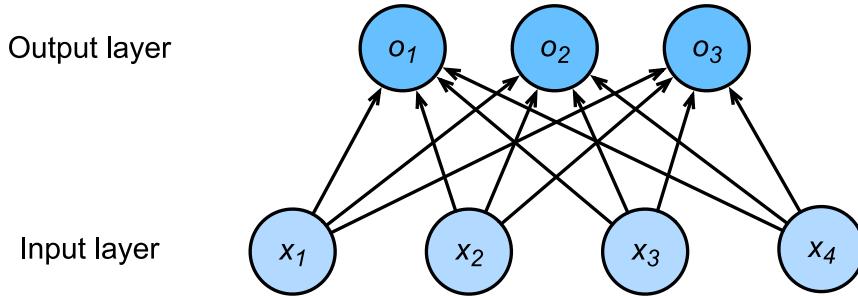


Fig. 5.4.1: Softmax regression is a single-layer neural network.

### Softmax Operation

To express the model more compactly, we can use linear algebra notation. In vector form, we arrive at  $\mathbf{o} = \mathbf{W}\mathbf{x} + \mathbf{b}$ , a form better suited both for mathematics, and for writing code. Note that we have gathered all of our weights into a  $3 \times 4$  matrix and that for a given example  $\mathbf{x}$  our outputs are given by a matrix vector product of our weights by our inputs plus our biases  $\mathbf{b}$ .

If we are interested in hard classifications, we need to convert these outputs into a discrete prediction. One straightforward way to do this is to treat the output values  $o_i$  as the relative confidence levels that the item belongs to each category  $i$ . Then we can choose the class with the largest output value as our prediction  $\text{argmax}_i o_i$ . For example, if  $o_1, o_2$ , and  $o_3$  are 0.1, 10, and 0.1, respectively, then we predict category 2, which represents “chicken”.

However, there are a few problems with using the output from the output layer directly. First, because the range of output values from the output layer is uncertain, it is difficult to judge the meaning of these values. For instance, the output value 10 from the previous example appears to indicate that we are *very confident* that the image category is *chicken*. But just how confident? Is it 100 times more likely to be a chicken than a dog or are we less confident?

Moreover how do we train this model. If the argmax matches the label, then we have no error at all! And if the argmax is not equal to the label, then no infinitesimal change in our weights will decrease our error. That takes gradient-based learning off the table.

We might like for our outputs to correspond to probabilities, but then we would need a way to guarantee that on new (unseen) data the probabilities would be nonnegative and sum up to 1. Moreover, we would need a training objective that encouraged the model to actually estimate *probabilities*. Fortunately, statisticians have conveniently invented a model called softmax logistic regression that does precisely this.

In order to ensure that our outputs are nonnegative and sum to 1, while requiring that our model remains differentiable, we subject the outputs of the linear portion of our model to a nonlinear *softmax* function:

$$\hat{\mathbf{y}} = \text{softmax}(\mathbf{o}) \quad \text{where} \quad \hat{y}_i = \frac{\exp(o_i)}{\sum_j \exp(o_j)} \quad (5.4.3)$$

It is easy to see  $\hat{y}_1 + \hat{y}_2 + \hat{y}_3 = 1$  with  $0 \leq \hat{y}_i \leq 1$  for all  $i$ . Thus,  $\hat{\mathbf{y}}$  is a proper probability distribution and the values of  $o$  now assume an easily quantifiable meaning. Note that we can still find the most likely class by

$$\hat{i}(\mathbf{o}) = \underset{i}{\text{argmax}} o_i = \underset{i}{\text{argmax}} \hat{y}_i \quad (5.4.4)$$

In short, the softmax operation preserves the orderings of its inputs, and thus does not alter the predicted category vs our simpler *argmax* model. However, it gives the outputs  $\mathbf{o}$  proper meaning: they are the pre-softmax values determining the probabilities assigned to each category. Summarizing it all in vector notation we get  $\mathbf{o}^{(i)} = \mathbf{W}\mathbf{x}^{(i)} + \mathbf{b}$  where  $\hat{\mathbf{y}}^{(i)} = \text{softmax}(\mathbf{o}^{(i)})$ .

### Vectorization for Minibatches

Again, to improve computational efficiency and take advantage of GPUs, we will typically carry out vector calculations for mini-batches of data. Assume that we are given a mini-batch  $\mathbf{X}$  of examples with dimensionality  $d$  and batch size  $n$ . Moreover, assume that we have  $q$  categories (outputs). Then the minibatch features  $\mathbf{X}$  are in  $\mathbb{R}^{n \times d}$ , weights  $\mathbf{W} \in \mathbb{R}^{d \times q}$  and the bias satisfies  $\mathbf{b} \in \mathbb{R}^q$ .

$$\begin{aligned}\mathbf{O} &= \mathbf{X}\mathbf{W} + \mathbf{b} \\ \hat{\mathbf{Y}} &= \text{softmax}(\mathbf{O})\end{aligned}\tag{5.4.5}$$

This accelerates the dominant operation into a matrix-matrix product  $\mathbf{WX}$  vs the matrix-vector products we would be executing if we processed one example at a time. The softmax itself can be computed by exponentiating all entries in  $\mathbf{O}$  and then normalizing them by the sum appropriately.

### 5.4.2 Loss Function

Now that we have some mechanism for outputting probabilities, we need to transform this into a measure of how accurate things are, i.e. we need a *loss function*. For this, we use the same concept that we already encountered in linear regression, namely likelihood maximization.

#### Log-Likelihood

The softmax function maps  $\mathbf{o}$  into a vector of probabilities corresponding to various outcomes, such as  $p(y = \text{cat}|\mathbf{x})$ . This allows us to compare the estimates with reality, simply by checking how well it predicted what we observe.

$$p(Y|X) = \prod_{i=1}^n p(y^{(i)}|x^{(i)}) \text{ and thus } -\log p(Y|X) = \sum_{i=1}^n -\log p(y^{(i)}|x^{(i)})\tag{5.4.6}$$

Maximizing  $p(Y|X)$  (and thus equivalently minimizing  $-\log p(Y|X)$ ) corresponds to predicting the label well. This yields the loss function (we dropped the superscript  $(i)$  to avoid notation clutter):

$$l = -\log p(y|x) = -\sum_j y_j \log \hat{y}_j\tag{5.4.7}$$

Here we used that by construction  $\hat{\mathbf{y}} = \text{softmax}(\mathbf{o})$  and moreover, that the vector  $\mathbf{y}$  consists of all zeroes but for the correct label, such as  $(1, 0, 0)$ . Hence the sum over all coordinates  $j$  vanishes for all but one term. Since all  $\hat{y}_j$  are probabilities, their logarithm is never larger than 0. Consequently, the loss function is minimized if we correctly predict  $y$  with *certainty*, i.e. if  $p(y|x) = 1$  for the correct label.

#### Softmax and Derivatives

Since the Softmax and the corresponding loss are so common, it is worth while understanding a bit better how it is computed. Plugging  $\mathbf{o}$  into the definition of the loss  $l$  and using the definition of the softmax we obtain:

$$l = -\sum_j y_j \log \hat{y}_j = \sum_j y_j \log \sum_k \exp(o_k) - \sum_j y_j o_j = \log \sum_k \exp(o_k) - \sum_j y_j o_j\tag{5.4.8}$$

To understand a bit better what is going on, consider the derivative with respect to  $o$ . We get

$$\partial_{o_j} l = \frac{\exp(o_j)}{\sum_k \exp(o_k)} - y_j = \text{softmax}(\mathbf{o})_j - y_j = \Pr(y = j|x) - y_j \quad (5.4.9)$$

In other words, the gradient is the difference between the probability assigned to the true class by our model, as expressed by the probability  $p(y|x)$ , and what actually happened, as expressed by  $y$ . In this sense, it is very similar to what we saw in regression, where the gradient was the difference between the observation  $y$  and estimate  $\hat{y}$ . This is not coincidence. In any [exponential family](#)<sup>60</sup> model, the gradients of the log-likelihood are given by precisely this term. This fact makes computing gradients easy in practice.

### Cross-Entropy Loss

Now consider the case where we don't just observe a single outcome but maybe, an entire distribution over outcomes. We can use the same representation as before for  $y$ . The only difference is that rather than a vector containing only binary entries, say  $(0, 0, 1)$ , we now have a generic probability vector, say  $(0.1, 0.2, 0.7)$ . The math that we used previously to define the loss  $l$  still works out fine, just that the interpretation is slightly more general. It is the expected value of the loss for a distribution over labels.

$$l(\mathbf{y}, \hat{\mathbf{y}}) = - \sum_j y_j \log \hat{y}_j \quad (5.4.10)$$

This loss is called the cross-entropy loss and it is one of the most commonly used losses for multiclass classification. To demystify its name we need some information theory. The following section can be skipped if needed.

### 5.4.3 Information Theory Basics

Information theory deals with the problem of encoding, decoding, transmitting and manipulating information (aka data), preferentially in as concise form as possible.

#### Entropy

A key concept is how many bits of information (or randomness) are contained in data. It can be measured as the [entropy](#)<sup>61</sup> of a distribution  $p$  via

$$H[p] = \sum_j -p(j) \log p(j) \quad (5.4.11)$$

One of the fundamental theorems of information theory states that in order to encode data drawn randomly from the distribution  $p$  we need at least  $H[p]$  ‘nats’ to encode it. If you wonder what a ‘nat’ is, it is the equivalent of bit but when using a code with base  $e$  rather than one with base 2. One nat is  $\frac{1}{\log(2)} \approx 1.44$  bit.  $H[p]/\log 2$  is often also called the binary entropy.

To make this all a bit more theoretical consider the following:  $p(1) = \frac{1}{2}$  whereas  $p(2) = p(3) = \frac{1}{4}$ . In this case we can easily design an optimal code for data drawn from this distribution, by using 0 to encode 1, 10 for 2 and 11 for 3. The expected number of bit is  $1.5 = 0.5 * 1 + 0.25 * 2 + 0.25 * 2$ . It is easy to check that this is the same as the binary entropy  $H[p]/\log 2$ .

<sup>60</sup> [https://en.wikipedia.org/wiki/Exponential\\_family](https://en.wikipedia.org/wiki/Exponential_family)

<sup>61</sup> [https://en.wikipedia.org/wiki/Entropy\\_\(information\\_theory\)](https://en.wikipedia.org/wiki/Entropy_(information_theory))

## Kullback Leibler Divergence

One way of measuring the difference between two distributions arises directly from the entropy. Since  $H[p]$  is the minimum number of bits that we need to encode data drawn from  $p$ , we could ask how well it is encoded if we pick the ‘wrong’ distribution  $q$ . The amount of extra bits that we need to encode  $q$  gives us some idea of how different these two distributions are. Let us compute this directly - recall that to encode  $j$  using an optimal code for  $q$  would cost  $-\log q(j)$  nats, and we need to use this in  $p(j)$  of all cases. Hence we have

$$D(p\|q) = - \sum_j p(j) \log q(j) - H[p] = \sum_j p(j) \log \frac{p(j)}{q(j)} \quad (5.4.12)$$

Note that minimizing  $D(p\|q)$  with respect to  $q$  is equivalent to minimizing the cross-entropy loss. This can be seen directly by dropping  $H[p]$  which doesn’t depend on  $q$ . We thus showed that softmax regression tries to minimize the surprise (and thus the number of bits) we experience when seeing the true label  $y$  rather than our prediction  $\hat{y}$ .

### 5.4.4 Model Prediction and Evaluation

After training the softmax regression model, given any example features, we can predict the probability of each output category. Normally, we use the category with the highest predicted probability as the output category. The prediction is correct if it is consistent with the actual category (label). In the next part of the experiment, we will use accuracy to evaluate the model’s performance. This is equal to the ratio between the number of correct predictions and the total number of predictions.

### 5.4.5 Summary

- We introduced the softmax operation which takes a vector maps it into probabilities.
- Softmax regression applies to classification problems. It uses the probability distribution of the output category in the softmax operation.
- Cross entropy is a good measure of the difference between two probability distributions. It measures the number of bits needed to encode the data given our model.

### 5.4.6 Exercises

1. Show that the Kullback-Leibler divergence  $D(p\|q)$  is nonnegative for all distributions  $p$  and  $q$ . Hint - use Jensen’s inequality, i.e. use the fact that  $-\log x$  is a convex function.
2. Show that  $\log \sum_j \exp(o_j)$  is a convex function in  $o$ .
3. We can explore the connection between exponential families and the softmax in some more depth
  - Compute the second derivative of the cross-entropy loss  $l(y, \hat{y})$  for the softmax.
  - Compute the variance of the distribution given by  $\text{softmax}(o)$  and show that it matches the second derivative computed above.
4. Assume that we three classes which occur with equal probability, i.e. the probability vector is  $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ .
  - What is the problem if we try to design a binary code for it? Can we match the entropy lower bound on the number of bits?
  - Can you design a better code. Hint - what happens if we try to encode two independent observations? What if we encode  $n$  observations jointly?

5. Softmax is a misnomer for the mapping introduced above (but everyone in deep learning uses it). The real softmax is defined as  $\text{RealSoftMax}(a, b) = \log(\exp(a) + \exp(b))$ .

- Prove that  $\text{RealSoftMax}(a, b) > \max(a, b)$ .
- Prove that this holds for  $\lambda^{-1}\text{RealSoftMax}(\lambda a, \lambda b)$ , provided that  $\lambda > 0$ .
- Show that for  $\lambda \rightarrow \infty$  we have  $\lambda^{-1}\text{RealSoftMax}(\lambda a, \lambda b) \rightarrow \max(a, b)$ .
- What does the soft-min look like?
- Extend this to more than two numbers.

#### 5.4.7 Scan the QR Code to Discuss<sup>62</sup>



## 5.5 Image Classification Data (Fashion-MNIST)

In Section 4.5 we trained a naive Bayes classifier on MNIST [34] introduced in 1998. Despite its popularity, MNIST is considered as a simple dataset, on which even simple models achieve classification accuracy over 95%. It is hard to spot the differences between better models and weaker ones. In order to get a better intuition, we will use the qualitatively similar, but comparatively complex Fashion-MNIST dataset [67] came out in 2017.

### 5.5.1 Getting the Data

First, import the packages or modules required in this section.

```
%matplotlib inline
import d2l
from mxnet import gluon
import sys
```

Again, Gluon provides a similar `FashionMNIST` class to download and load this dataset.

```
mnist_train = gluon.data.vision.FashionMNIST(train=True)
mnist_test = gluon.data.vision.FashionMNIST(train=False)
```

The number of images for each category in the training set and the testing set is 6,000 and 1,000, respectively. Since there are 10 categories, the numbers of examples in the training set and the test set are 60,000 and 10,000, respectively.

```
len(mnist_train), len(mnist_test)
```

<sup>62</sup> <https://discuss.mxnet.io/t/2334>

(60000, 10000)

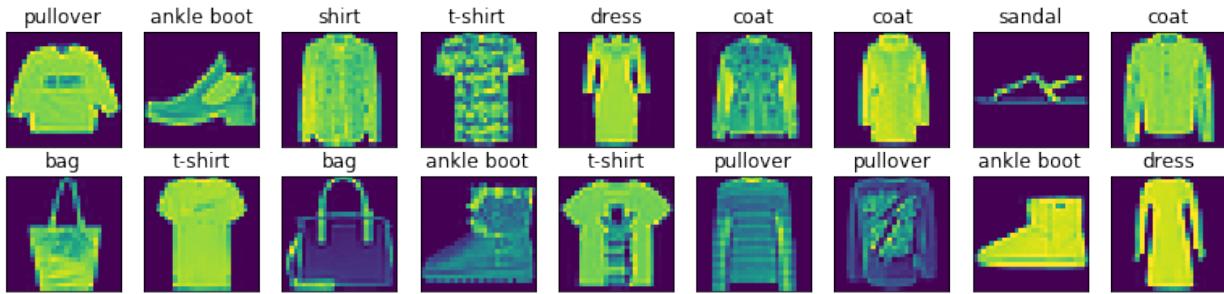
Please refer to [Section 4.5](#) for more detailed explanations about accessing these examples and the example format.

There are 10 categories in Fashion-MNIST: t-shirt, trousers, pullover, dress, coat, sandal, shirt, sneaker, bag and ankle boot. The following function can convert a numeric label into a corresponding text label.

```
# Save to the d2l package.
def get_fashion_mnist_labels(labels):
    text_labels = ['t-shirt', 'trouser', 'pullover', 'dress', 'coat',
                  'sandal', 'shirt', 'sneaker', 'bag', 'ankle boot']
    return [text_labels[int(i)] for i in labels]
```

Next, let's take a look at the image contents and text labels for the first few examples in the training data set.

```
X, y = mnist_train[:18]
d2l.show_images(X.squeeze(axis=-1), 2, 9, titles=get_fashion_mnist_labels(y));
```



### 5.5.2 Reading a Minibatch

To make our life easier when reading from the training and test sets we use a `DataLoader` rather than creating one from scratch, as we did in [Section 5.2](#). Recall that a data loader reads a mini-batch of data with an example number of `batch_size` each time.

In practice, reading data can often be a significant performance bottleneck for training, especially when the model is simple or when the computer is fast. A handy feature of Gluon's `DataLoader` is the ability to use multiple processes to speed up data reading (not currently supported on Windows). For instance, we can set aside 4 processes to read the data (via `num_workers`).

```
# Save to the d2l package.
def get_dataloader_workers(num_workers=4):
    # 0 means no additional process is used to speed up the reading of data.
    if sys.platform.startswith('win'):
        return 0
    else:
        return num_workers
```

In addition, we convert the image data from `uint8` to 32-bit floating point numbers using the `ToTensor` class. Beyond that, it will divide all numbers by 255 so that all pixels have values between 0 and 1. The `ToTensor` class also moves the image channel from the last dimension to the first dimension to facilitate the convolutional neural network calculations introduced later. Through the `transform_first` function of the

data set, we apply the transformation of `ToTensor` to the first element of each data example (image and label), i.e., the image.

```
batch_size = 256
transformer = gluon.data.vision.transforms.ToTensor()
train_iter = gluon.data.DataLoader(mnist_train.transform_first(transformer),
                                   batch_size, shuffle=True,
                                   num_workers=get_dataloader_workers())
```

Let's look at the time it takes to read the training data.

```
timer = d2l.Timer()
for X, y in train_iter:
    continue
'%.2f sec' % timer.stop()
```

'1.25 sec'

### 5.5.3 Put all Things Together

Now we define the `load_data_fashion_mnist` function that obtains and reads the Fashion-MNIST data set. It returns the data iterators for both the training set and validation set. In addition, it accepts an optional argument to resize images to another shape.

```
# Save to the d2l package.
def load_data_fashion_mnist(batch_size, resize=None):
    """Download the Fashion-MNIST dataset and then load into memory."""
    dataset = gluon.data.vision
    trans = [dataset.transforms.Resize(resize)] if resize else []
    trans.append(dataset.transforms.ToTensor())
    trans = dataset.transforms.Compose(trans)
    mnist_train = dataset.FashionMNIST(train=True).transform_first(trans)
    mnist_test = dataset.FashionMNIST(train=False).transform_first(trans)
    return (gluon.data.DataLoader(mnist_train, batch_size, shuffle=True,
                                  num_workers=get_dataloader_workers()),
            gluon.data.DataLoader(mnist_test, batch_size, shuffle=False,
                                  num_workers=get_dataloader_workers()))
```

Verify image resizing works.

```
train_iter, test_iter = load_data_fashion_mnist(32, (64, 64))
for X, y in train_iter:
    print(X.shape)
    break
```

(32, 1, 64, 64)

### 5.5.4 Summary

- Fashion-MNIST is an apparel classification data set containing 10 categories, which we will use to test the performance of different algorithms in later chapters.

- We store the shape of image using height and width of  $h$  and  $w$  pixels, respectively, as  $h \times w$  or `(h, w)`.
- Data iterators are a key component for efficient performance. Use existing ones if available.

### 5.5.5 Exercises

1. Does reducing `batch_size` (for instance, to 1) affect read performance?
2. For non-Windows users, try modifying `num_workers` to see how it affects read performance.
3. Use the MXNet documentation to see which other datasets are available in `mxnet.gluon.data.vision`.
4. Use the MXNet documentation to see which other transformations are available in `mxnet.gluon.data.vision.transforms`.

### 5.5.6 Scan the QR Code to Discuss<sup>63</sup>



## 5.6 Implementation of Softmax Regression from Scratch

Just as we implemented linear regression from scratch, we believe that multiclass logistic (softmax) regression is similarly fundamental and you ought to know the gory details of how to implement it from scratch. As with linear regression, after doing things by hand we will breeze through an implementation in Gluon for comparison. To begin, let's import our packages (only `autograd`, `nd` are needed here because we will be doing the heavy lifting ourselves.)

```
import d2l
from mxnet import autograd, nd, gluon
from IPython import display
```

We will work with the Fashion-MNIST dataset just introduced, cuing up an iterator with batch size 256.

```
batch_size = 256
train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size)
```

### 5.6.1 Initialize Model Parameters

Just as in linear regression, we represent each example as a vector. Since each example is a  $28 \times 28$  image, we can flatten each example, treating them as 784 dimensional vectors. In the future, we'll talk about more sophisticated strategies for exploiting the spatial structure in images, but for now we treat each pixel location as just another feature.

---

<sup>63</sup> <https://discuss.mxnet.io/t/2335>

Recall that in softmax regression, we have as many outputs as there are categories. Because our dataset has 10 categories, our network will have an output dimension of 10. Consequently, our weights will constitute a  $784 \times 10$  matrix and the biases will constitute a  $1 \times 10$  vector. As with linear regression, we will initialize our weights  $W$  with Gaussian noise and our biases to take the initial value 0.

```
num_inputs = 784
num_outputs = 10

W = nd.random.normal(scale=0.01, shape=(num_inputs, num_outputs))
b = nd.zeros(num_outputs)
```

Recall that we need to *attach gradients* to the model parameters. More literally, we are allocating memory for future gradients to be stored and notifying MXNet that we want gradients to be calculated with respect to these parameters in the first place.

```
W.attach_grad()
b.attach_grad()
```

## 5.6.2 The Softmax

Before implementing the softmax regression model, let's briefly review how operators such as `sum` work along specific dimensions in an NDArray. Given a matrix  $X$  we can sum over all elements (default) or only over elements in the same column (`axis=0`) or the same row (`axis=1`). Note that if  $X$  is an array with shape  $(2, 3)$  and we sum over the columns (`X.sum(axis=0)`), the result will be a (1D) vector with shape  $(3,)$ . If we want to keep the number of axes in the original array (resulting in a 2D array with shape  $(1, 3)$ ), rather than collapsing out the dimension that we summed over we can specify `keepdims=True` when invoking `sum`.

```
X = nd.array([[1, 2, 3], [4, 5, 6]])
X.sum(axis=0, keepdims=True), X.sum(axis=1, keepdims=True)
```

```
(  
 [[5. 7. 9.]]  
<NDArray 1x3 @cpu(0)>,  
 [[ 6.]  
 [15.]]  
<NDArray 2x1 @cpu(0)>)
```

We are now ready to implement the softmax function. Recall that softmax consists of two steps: First, we exponentiate each term (using `exp`). Then, we sum over each row (we have one row per example in the batch) to get the normalization constants for each example. Finally, we divide each row by its normalization constant, ensuring that the result sums to 1. Before looking at the code, let's recall what this looks expressed as an equation:

$$\text{softmax}(\mathbf{X})_{ij} = \frac{\exp(X_{ij})}{\sum_k \exp(X_{ik})} \quad (5.6.1)$$

The denominator, or normalization constant, is also sometimes called the partition function (and its logarithm the log-partition function). The origins of that name are in statistical physics<sup>64</sup> where a related equation models the distribution over an ensemble of particles).

<sup>64</sup> [https://en.wikipedia.org/wiki/Partition\\_function\\_\(statistical\\_mechanics\)](https://en.wikipedia.org/wiki/Partition_function_(statistical_mechanics))

```
def softmax(X):
    X_exp = X.exp()
    partition = X_exp.sum(axis=1, keepdims=True)
    return X_exp / partition # The broadcast mechanism is applied here
```

As you can see, for any random input, we turn each element into a non-negative number. Moreover, each row sums up to 1, as is required for a probability. Note that while this looks correct mathematically, we were a bit sloppy in our implementation because failed to take precautions against numerical overflow or underflow due to large (or very small) elements of the matrix, as we did in [Section 4.5](#).

```
X = nd.random.normal(shape=(2, 5))
X_prob = softmax(X)
X_prob, X_prob.sum(axis=1)
```

```
(([[0.21324193 0.33961776 0.1239742 0.27106097 0.05210521]
 [0.11462264 0.3461234 0.19401033 0.29583326 0.04941036]]
<NDArray 2x5 @cpu(0)>,
 [1.0000001 1.])
<NDArray 2 @cpu(0)>)
```

### 5.6.3 The Model

Now that we have defined the softmax operation, we can implement the softmax regression model. The below code defines the forward pass through the network. Note that we flatten each original image in the batch into a vector with length `num_inputs` with the `reshape` function before passing the data through our model.

```
def net(X):
    return softmax(nd.dot(X.reshape((-1, num_inputs)), W) + b)
```

### 5.6.4 The Loss Function

Next, we need to implement the cross-entropy loss function, introduced in [Section 5.4](#). This may be the most common loss function in all of deep learning because, at the moment, classification problems far outnumber regression problems.

Recall that cross-entropy takes the negative log likelihood of the predicted probability assigned to the true label  $-\log p(y|x)$ . Rather than iterating over the predictions with a Python `for` loop (which tends to be inefficient), we can use the `pick` function which allows us to select the appropriate terms from the matrix of softmax entries easily. Below, we illustrate the `pick` function on a toy example, with 3 categories and 2 examples.

```
y_hat = nd.array([[0.1, 0.3, 0.6], [0.3, 0.2, 0.5]])
y = nd.array([0, 2], dtype='int32')
nd.pick(y_hat, y)
```

```
[0.1 0.5]
<NDArray 2 @cpu(0)>
```

Now we can implement the cross-entropy loss function efficiently with just one line of code.

```
def cross_entropy(y_hat, y):
    return - nd.pick(y_hat, y).log()
```

### 5.6.5 Classification Accuracy

Given the predicted probability distribution `y_hat`, we typically choose the class with highest predicted probability whenever we must output a *hard* prediction. Indeed, many applications require that we make a choice. Gmail must categorize an email into Primary, Social, Updates, or Forums. It might estimate probabilities internally, but at the end of the day it has to choose one among the categories.

When predictions are consistent with the actual category `y`, they are correct. The classification accuracy is the fraction of all predictions that are correct. Although we cannot optimize accuracy directly (it is not differentiable), it's often the performance metric that we care most about, and we will nearly always report it when training classifiers.

To compute accuracy we do the following: First, we execute `y_hat.argmax(axis=1)` to gather the predicted classes (given by the indices for the largest entries each row). The result has the same shape as the variable `y`. Now we just need to check how frequently the two match. Since the equality operator `==` is datatype-sensitive (e.g. an `int` and a `float32` are never equal), we also need to convert both to the same type (we pick `float32`). The result is an NDArray containing entries of 0 (false) and 1 (true). Taking the mean yields the desired result.

```
# Save to the d2l package.
def accuracy(y_hat, y):
    return (y_hat.argmax(axis=1) == y.astype('float32')).sum().asscalar()
```

We will continue to use the variables `y_hat` and `y` defined in the `pick` function, as the predicted probability distribution and label, respectively. We can see that the first example's prediction category is 2 (the largest element of the row is 0.6 with an index of 2), which is inconsistent with the actual label, 0. The second example's prediction category is 2 (the largest element of the row is 0.5 with an index of 2), which is consistent with the actual label, 2. Therefore, the classification accuracy rate for these two examples is 0.5.

```
accuracy(y_hat, y) / len(y)
```

```
0.5
```

Similarly, we can evaluate the accuracy for model `net` on the data set (accessed via `data_iter`).

```
# Save to the d2l package.
def evaluate_accuracy(net, data_iter):
    metric = Accumulator(2) # num_corrected_examples, num_examples
    for X, y in data_iter:
        y = y.astype('float32')
        metric.add(accuracy(net(X), y), y.size)
    return metric[0] / metric[1]
```

Here `Accumulator` is a utility class to accumulated sum over multiple numbers.

```
# Save to the d2l package.
class Accumulator(object):
    """Sum a list of numbers over time"""
    def __init__(self, n):
        self.data = [0.0] * n
```

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```

def add(self, *args):
    self.data = [a+b for a, b in zip(self.data, args)]
def reset(self):
    self.data = [0] * len(self.data)
def __getitem__(self, i):
    return self.data[i]

```

Because we initialized the `net` model with random weights, the accuracy of this model should be close to random guessing, i.e. 0.1 for 10 classes.

```
evaluate_accuracy(net, test_iter)
```

```
0.0925
```

## 5.6.6 Model Training

The training loop for softmax regression should look strikingly familiar if you read through our implementation of linear regression in [Section 5.2](#). Here we refactor the implementation to make it reusable. First, we define a function to train for one data epoch. Note that `updater` is general function to update the model parameters, which accepts the batch size as an argument. It can be either a wrapper of `d2l.sgd` or a Gluon trainer.

```

# Save to the d2l package.
def train_epoch_ch3(net, train_iter, loss, updater):
    metric = Accumulator(3) # train_loss_sum, train_acc_sum, num_examples
    if isinstance(updater, gluon.Trainer):
        updater = updater.step
    for X, y in train_iter:
        # compute gradients and update parameters
        with autograd.record():
            y_hat = net(X)
            l = loss(y_hat, y)
            l.backward()
            updater(X.shape[0])
            metric.add(l.sum().asscalar(), accuracy(y_hat, y), y.size)
    # Return training loss and training accuracy
    return metric[0]/metric[2], metric[1]/metric[2]

```

Before showing the implementation of the training function, we define a utility class that draw data in animation. Again, it aims to simplify the codes in later chapters.

```

# Save to the d2l package.
class Animator(object):
    def __init__(self, xlabel=None, ylabel=None, legend=[], xlim=None,
                 ylim=None, xscale='linear', yscale='linear', fmts=None,
                 nrows=1, ncols=1, figsize=(3.5, 2.5)):
        """Incrementally plot multiple lines."""
        d2l.use_svg_display()
        self.fig, self.axes = d2l.plt.subplots(nrows, ncols, figsize=figsize)
        if nrows * ncols == 1: self.axes = [self.axes,]
        # use a lambda to capture arguments

```

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```

self.config_axes = lambda : d2l.set_axes(
    self.axes[0], xlabel, ylabel, xlim, ylim, xscale, yscale, legend)
self.X, self.Y, self.fmts = None, None, fmts

def add(self, x, y):
    """Add multiple data points into the figure."""
    if not hasattr(y, "__len__"): y = [y]
    n = len(y)
    if not hasattr(x, "__len__"): x = [x] * n
    if not self.X: self.X = [[] for _ in range(n)]
    if not self.Y: self.Y = [[] for _ in range(n)]
    if not self.fmts: self.fmts = ['-' * n]
    for i, (a, b) in enumerate(zip(x, y)):
        if a is not None and b is not None:
            self.X[i].append(a)
            self.Y[i].append(b)
    self.axes[0].cla()
    for x, y, fmt in zip(self.X, self.Y, self.fmts):
        self.axes[0].plot(x, y, fmt)
    self.config_axes()
    display.display(self.fig)
    display.clear_output(wait=True)

```

The training function then runs multiple epochs and visualize the training progress.

```

# Save to the d2l package.
def train_ch3(net, train_iter, test_iter, loss, num_epochs, updater):
    trains, test_accs = [], []
    animator = Animator(xlabel='epoch', xlim=[1, num_epochs],
                         ylim=[0.3, 0.9],
                         legend=['train loss', 'train acc', 'test acc'])
    for epoch in range(num_epochs):
        train_metrics = train_epoch_ch3(net, train_iter, loss, updater)
        test_acc = evaluate_accuracy(net, test_iter)
        animator.add(epoch+1, train_metrics+(test_acc,))

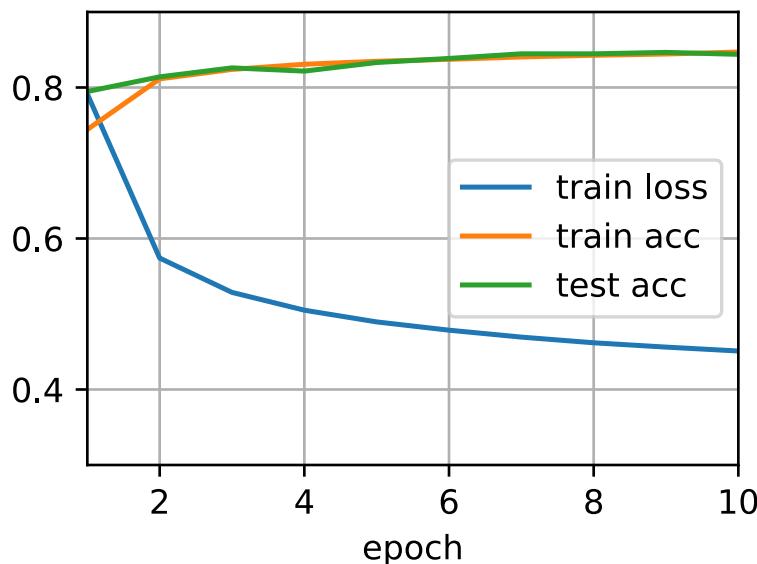
```

Again, we use the mini-batch stochastic gradient descent to optimize the loss function of the model. Note that the number of epochs (`num_epochs`), and learning rate (`lr`) are both adjustable hyper-parameters. By changing their values, we may be able to increase the classification accuracy of the model. In practice we'll want to split our data three ways into training, validation, and test data, using the validation data to choose the best values of our hyperparameters.

```

num_epochs, lr = 10, 0.1
updater = lambda batch_size: d2l.sgd([W, b], lr, batch_size)
train_ch3(net, train_iter, test_iter, cross_entropy, num_epochs, updater)

```

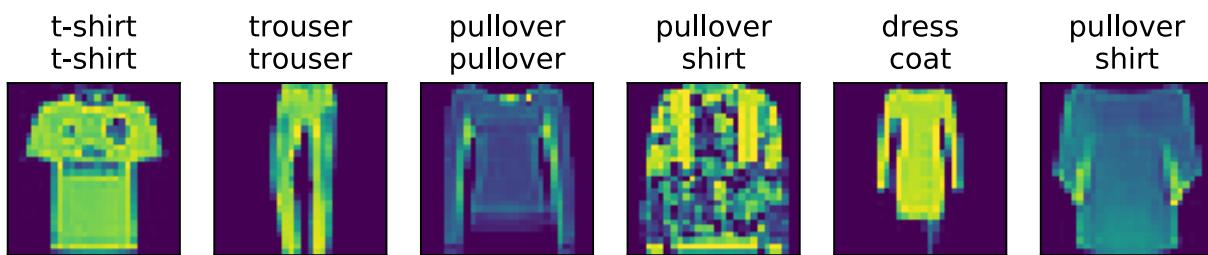


### 5.6.7 Prediction

Now that training is complete, our model is ready to classify some images. Given a series of images, we will compare their actual labels (first line of text output) and the model predictions (second line of text output).

```
# Save to the d2l package.
def predict_ch3(net, test_iter, n=6):
    for X, y in test_iter:
        break
    trues = d2l.get_fashion_mnist_labels(y.asnumpy())
    preds = d2l.get_fashion_mnist_labels(net(X).argmax(axis=1).asnumpy())
    titles = [true+'\n'+ pred for true, pred in zip(trues, preds)]
    d2l.show_images(X[0:n].reshape((n,28,28)), 1, n, titles=titles[0:n])

predict_ch3(net, test_iter)
```



### 5.6.8 Summary

With softmax regression, we can train models for multi-category classification. The training loop is very similar to that in linear regression: retrieve and read data, define models and loss functions, then train models using optimization algorithms. As you'll soon find out, most common deep learning models have similar training procedures.

### 5.6.9 Exercises

1. In this section, we directly implemented the softmax function based on the mathematical definition of the softmax operation. What problems might this cause (hint - try to calculate the size of  $\exp(50)$ )?
2. The function `cross_entropy` in this section is implemented according to the definition of the cross-entropy loss function. What could be the problem with this implementation (hint - consider the domain of the logarithm)?
3. What solutions you can think of to fix the two problems above?
4. Is it always a good idea to return the most likely label. E.g. would you do this for medical diagnosis?
5. Assume that we want to use softmax regression to predict the next word based on some features. What are some problems that might arise from a large vocabulary?

### 5.6.10 Scan the QR Code to Discuss<sup>65</sup>



## 5.7 Concise Implementation of Softmax Regression

Just as Gluon made it much easier to implement linear regression in Section 5.3, we'll find it similarly (or possibly more) convenient for implementing classification models. Again, we begin with our import ritual.

```
import d2l
from mxnet import gluon, init
from mxnet.gluon import nn
```

Let's stick with the Fashion-MNIST dataset and keep the batch size at 256 as in the last section.

```
batch_size = 256
train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size)
```

### 5.7.1 Initialize Model Parameters

As mentioned in Section 5.4, the output layer of softmax regression is a fully connected (`Dense`) layer. Therefore, to implement our model, we just need to add one `Dense` layer with 10 outputs to our `Sequential`. Again, here, the `Sequential` isn't really necessary, but we might as well form the habit since it will be ubiquitous when implementing deep models. Again, we initialize the weights at random with zero mean and standard deviation 0.01.

```
net = nn.Sequential()
net.add(nn.Dense(10))
net.initialize(init.Normal(sigma=0.01))
```

<sup>65</sup> <https://discuss.mxnet.io/t/2336>

## 5.7.2 The Softmax

In the previous example, we calculated our model's output and then ran this output through the cross-entropy loss. At its heart it uses `-nd.pick(y_hat, y).log()`. Mathematically, that's a perfectly reasonable thing to do. However, computationally, things can get hairy when dealing with exponentiation due to numerical stability issues, a matter we've already discussed a few times (e.g. in [Section 4.5](#)) and in the problem set of the previous chapter). Recall that the softmax function calculates  $\hat{y}_j = \frac{e^{z_j}}{\sum_{i=1}^n e^{z_i}}$ , where  $\hat{y}_j$  is the j-th element of `yhat` and  $z_j$  is the j-th element of the input `y_linear` variable, as computed by the softmax.

If some of the  $z_i$  are very large (i.e. very positive),  $e^{z_i}$  might be larger than the largest number we can have for certain types of `float` (i.e. overflow). This would make the denominator (and/or numerator) `inf` and we get zero, or `inf`, or `nan` for  $\hat{y}_j$ . In any case, we won't get a well-defined return value for `cross_entropy`. This is the reason we subtract  $\max(z_i)$  from all  $z_i$  first in `softmax` function. You can verify that this shifting in  $z_i$  will not change the return value of `softmax`.

After the above subtraction/ normalization step, it is possible that  $z_j$  is very negative. Thus,  $e^{z_j}$  will be very close to zero and might be rounded to zero due to finite precision (i.e underflow), which makes  $\hat{y}_j$  zero and we get `-inf` for  $\log(\hat{y}_j)$ . A few steps down the road in backpropagation, we start to get horrific not-a-number (`nan`) results printed to screen.

Our salvation is that even though we're computing these exponential functions, we ultimately plan to take their log in the cross-entropy functions. It turns out that by combining these two operators `softmax` and `cross_entropy` together, we can escape the numerical stability issues that might otherwise plague us during backpropagation. As shown in the equation below, we avoided calculating  $e^{z_j}$  but directly used  $z_j$  due to  $\log(\exp(\cdot))$ .

$$\begin{aligned}\log(\hat{y}_j) &= \log\left(\frac{e^{z_j}}{\sum_{i=1}^n e^{z_i}}\right) \\ &= \log(e^{z_j}) - \log\left(\sum_{i=1}^n e^{z_i}\right) \\ &= z_j - \log\left(\sum_{i=1}^n e^{z_i}\right)\end{aligned}\tag{5.7.1}$$

We'll want to keep the conventional softmax function handy in case we ever want to evaluate the probabilities output by our model. But instead of passing softmax probabilities into our new loss function, we'll just pass  $\hat{y}$  and compute the softmax and its log all at once inside the `softmax_cross_entropy` loss function, which does smart things like the log-sum-exp trick (see on [Wikipedia<sup>66</sup>](#)).

```
loss = gluon.loss.SoftmaxCrossEntropyLoss()
```

## 5.7.3 Optimization Algorithm

We use the mini-batch random gradient descent with a learning rate of 0.1 as the optimization algorithm. Note that this is the same choice as for linear regression and it illustrates the general applicability of the optimizers.

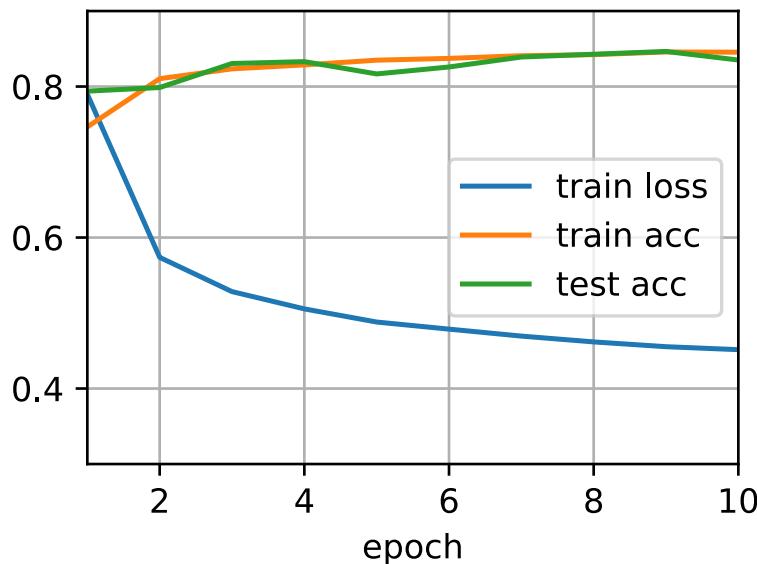
```
trainer = gluon.Trainer(net.collect_params(), 'sgd', {'learning_rate': 0.1})
```

## 5.7.4 Training

Next, we use the training functions defined in the last section to train a model.

<sup>66</sup> <https://en.wikipedia.org/wiki/LogSumExp>

```
num_epochs = 10
d2l.train_ch3(net, train_iter, test_iter, loss, num_epochs, trainer)
```



Just as before, this algorithm converges to a solution that achieves an accuracy of 83.7%, albeit this time with a lot fewer lines of code than before. Note that in many cases, Gluon takes specific precautions in addition to the most well-known tricks for ensuring numerical stability. This saves us from many common pitfalls that might befall us if we were to code all of our models from scratch.

### 5.7.5 Exercises

1. Try adjusting the hyper-parameters, such as batch size, epoch, and learning rate, to see what the results are.
2. Why might the test accuracy decrease again after a while? How could we fix this?

### 5.7.6 Scan the QR Code to Discuss<sup>67</sup>



<sup>67</sup> <https://discuss.mxnet.io/t/2337>



## MULTILAYER PERCEPTRONS

In this chapter, we will introduce your first truly *deep* networks. The simplest deep networks are called multilayer perceptrons, and they consist of many layers of neurons each fully connected to those in the layer below (from which they receive input) and those above (which they, in turn, influence). When we train high-capacity models we run the risk of overfitting. Thus, we will need to provide your first rigorous introduction to the notions of overfitting, underfitting, and capacity control. To help you combat these problems, we will introduce regularization techniques such as dropout and weight decay. We will also discuss issues relating to numerical stability and parameter initialization that are key to successfully training deep networks. Throughout, we focus on applying models to real data, aiming to give the reader a firm grasp not just of the concepts but also of the practice of using deep networks. We punt matters relating to the computational performance, scalability and efficiency of our models to subsequent chapters.

### 6.1 Multilayer Perceptron

In the previous chapters, we showed how you could implement multiclass logistic regression (also called softmax regression) for classifying images of clothing into the 10 possible categories. To get there, we had to learn how to wrangle data, coerce our outputs into a valid probability distribution (via `softmax`), how to apply an appropriate loss function, and how to optimize over our parameters. Now that we've covered these preliminaries, we are free to focus our attention on the more exciting enterprise of designing powerful models using deep neural networks.

#### 6.1.1 Hidden Layers

Recall that for linear regression and softmax regression, we mapped our inputs directly to our outputs via a single linear transformation:

$$\hat{\mathbf{o}} = \text{softmax}(\mathbf{W}\mathbf{x} + \mathbf{b}) \quad (6.1.1)$$

If our labels really were related to our input data by an approximately linear function, then this approach would be perfect. But linearity is a *strong assumption*. Linearity implies that for whatever target value we are trying to predict, increasing the value of each of our inputs should either drive the value of the output up or drive it down, irrespective of the value of the other inputs.

Sometimes this makes sense! Say we are trying to predict whether an individual will or will not repay a loan. We might reasonably imagine that all else being equal, an applicant with a higher income would be more likely to repay than one with a lower income. In these cases, linear models might perform well, and they might even be hard to beat.

But what about classifying images in FashionMNIST? Should increasing the intensity of the pixel at location (13,17) always increase the likelihood that the image depicts a pocketbook? That seems ridiculous because

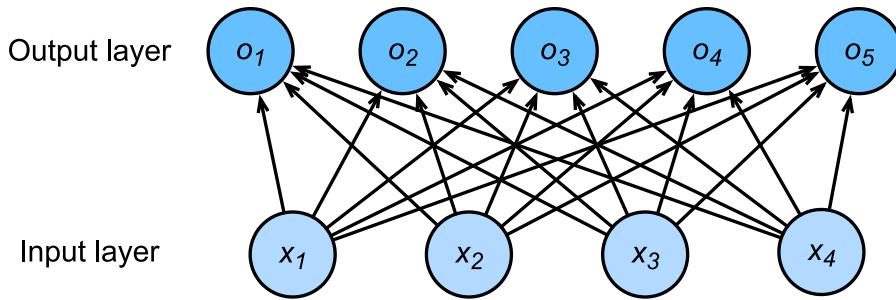


Fig. 6.1.1: Single layer perceptron with 5 output units.

we all know that you cannot make sense out of an image without accounting for the interactions among pixels.

### From one to many

As another case, consider trying to classify images based on whether they depict *cats* or *dogs* given black-and-white images.

If we use a linear model, we'd basically be saying that for each pixel, increasing its value (making it more white) must always increase the probability that the image depicts a dog or must always increase the probability that the image depicts a cat. We would be making the absurd assumption that the only requirement for differentiating cats vs. dogs is to assess how bright they are. That approach is doomed to fail in a work that contains both black dogs and black cats, and both white dogs and white cats.

Teasing out what is depicted in an image generally requires allowing more complex relationships between our inputs and outputs. Thus we need models capable of discovering patterns that might be characterized by interactions among the many features. We can over come these limitations of linear models and handle a more general class of functions by incorporating one or more hidden layers. The easiest way to do this is to stack many layers of neurons on top of each other. Each layer feeds into the layer above it, until we generate an output. This architecture is commonly called a *multilayer perceptron*, often abbreviated as *MLP*. The neural network diagram for an MLP looks like this:

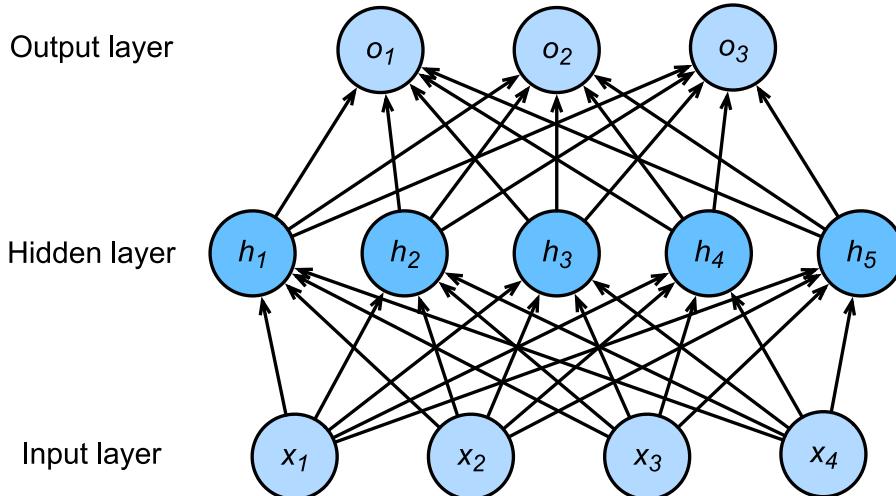


Fig. 6.1.2: Multilayer perceptron with hidden layers. This example contains a hidden layer with 5 hidden units in it.

The multilayer perceptron above has 4 inputs and 3 outputs, and the hidden layer in the middle contains 5 hidden units. Since the input layer does not involve any calculations, building this network would consist of implementing 2 layers of computation. The neurons in the input layer are fully connected to the inputs in the hidden layer. Likewise, the neurons in the hidden layer are fully connected to the neurons in the output layer.

### From linear to nonlinear

We can write out the calculations that define this one-hidden-layer MLP in mathematical notation as follows:

$$\begin{aligned}\mathbf{h} &= \mathbf{W}_1 \mathbf{x} + \mathbf{b}_1 \\ \mathbf{o} &= \mathbf{W}_2 \mathbf{h} + \mathbf{b}_2 \\ \hat{\mathbf{y}} &= \text{softmax}(\mathbf{o})\end{aligned}\tag{6.1.2}$$

By adding another layer, we have added two new sets of parameters, but what have we gained in exchange? In the model defined above, we do not achieve anything for our troubles!

That's because our hidden units are just a linear function of the inputs and the outputs (pre-softmax) are just a linear function of the hidden units. A linear function of a linear function is itself a linear function. That means that for any values of the weights, we could just collapse out the hidden layer yielding an equivalent single-layer model using  $\mathbf{W} = \mathbf{W}_2 \mathbf{W}_1$  and  $\mathbf{b} = \mathbf{W}_2 \mathbf{b}_1 + \mathbf{b}_2$ .

$$\mathbf{o} = \mathbf{W}_2 \mathbf{h} + \mathbf{b}_2 = \mathbf{W}_2(\mathbf{W}_1 \mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2 = (\mathbf{W}_2 \mathbf{W}_1) \mathbf{x} + (\mathbf{W}_2 \mathbf{b}_1 + \mathbf{b}_2) = \mathbf{W} \mathbf{x} + \mathbf{b}\tag{6.1.3}$$

In order to get a benefit from multilayer architectures, we need another key ingredient—a nonlinearity  $\sigma$  to be applied to each of the hidden units after each layer's linear transformation. The most popular choice for the nonlinearity these days is the rectified linear unit (ReLU)  $\max(x, 0)$ . After incorporating these non-linearities it becomes impossible to merge layers.

$$\begin{aligned}\mathbf{h} &= \sigma(\mathbf{W}_1 \mathbf{x} + \mathbf{b}_1) \\ \mathbf{o} &= \mathbf{W}_2 \mathbf{h} + \mathbf{b}_2 \\ \hat{\mathbf{y}} &= \text{softmax}(\mathbf{o})\end{aligned}\tag{6.1.4}$$

Clearly, we could continue stacking such hidden layers, e.g.  $\mathbf{h}_1 = \sigma(\mathbf{W}_1 \mathbf{x} + \mathbf{b}_1)$  and  $\mathbf{h}_2 = \sigma(\mathbf{W}_2 \mathbf{h}_1 + \mathbf{b}_2)$  on top of each other to obtain a true multilayer perceptron.

Multilayer perceptrons can account for complex interactions in the inputs because the hidden neurons depend on the values of each of the inputs. It's easy to design a hidden node that does arbitrary computation, such as, for instance, logical operations on its inputs. Moreover, for certain choices of the activation function it's widely known that multilayer perceptrons are universal approximators. That means that even for a single-hidden-layer neural network, with enough nodes, and the right set of weights, we can model any function at all! *Actually learning that function is the hard part.*

Moreover, just because a single-layer network *can* learn any function doesn't mean that you should try to solve all of your problems with single-layer networks. It turns out that we can approximate many functions much more compactly if we use deeper (vs wider) neural networks. We'll get more into the math in a subsequent chapter, but for now let's actually build an MLP. In this example, we'll implement a multilayer perceptron with two hidden layers and one output layer.

### Vectorization and mini-batch

As before, by the matrix  $\mathbf{X}$ , we denote a mini-batch of inputs. The calculations to produce outputs from an MLP with two hidden layers can thus be expressed:

$$\begin{aligned}\mathbf{H}_1 &= \sigma(\mathbf{X}_1 \mathbf{W}_1 + \mathbf{b}_1) \\ \mathbf{H}_2 &= \sigma(\mathbf{H}_1 \mathbf{W}_2 + \mathbf{b}_2) \\ \mathbf{O} &= \text{softmax}(\mathbf{H}_2 \mathbf{W}_3 + \mathbf{b}_3)\end{aligned}\tag{6.1.5}$$

With some abuse of notation, we define the nonlinearity  $\sigma$  to apply to its inputs on a row-wise fashion, i.e. one observation at a time. Note that we are also using the notation for *softmax* in the same way to denote a row-wise operation. Often, as in this chapter, the activation functions that we apply to hidden layers are not merely row-wise, but component wise. That means that after computing the linear portion of the layer, we can calculate each nodes activation without looking at the values taken by the other hidden units. This is true for most activation functions (the batch normalization operation will be introduced in Section 9.5 is a notable exception to that rule).

```
%matplotlib inline
import d2l
from mxnet import autograd, nd
```

### 6.1.2 Activation Functions

Because they are so fundamental to deep learning, before going further, let's take a brief look at some common activation functions.

#### ReLU Function

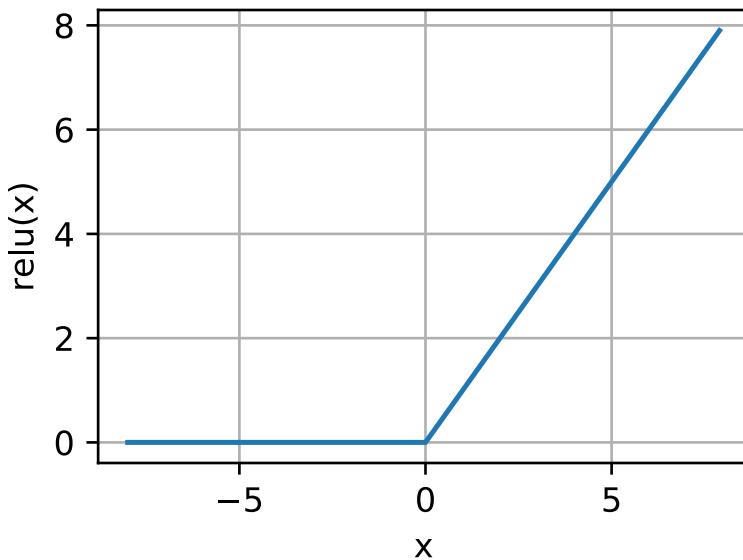
As stated above, the most popular choice, due to its simplicity of implementation and its efficacy in training is the rectified linear unit (ReLU). ReLUs provide a very simple nonlinear transformation. Given the element  $z$ , the function is defined as the maximum of that element and 0.

$$\text{ReLU}(z) = \max(z, 0). \quad (6.1.6)$$

It can be understood that the ReLU function retains only positive elements and discards negative elements (setting those nodes to 0). To get a better idea of what it looks like, we can plot it.

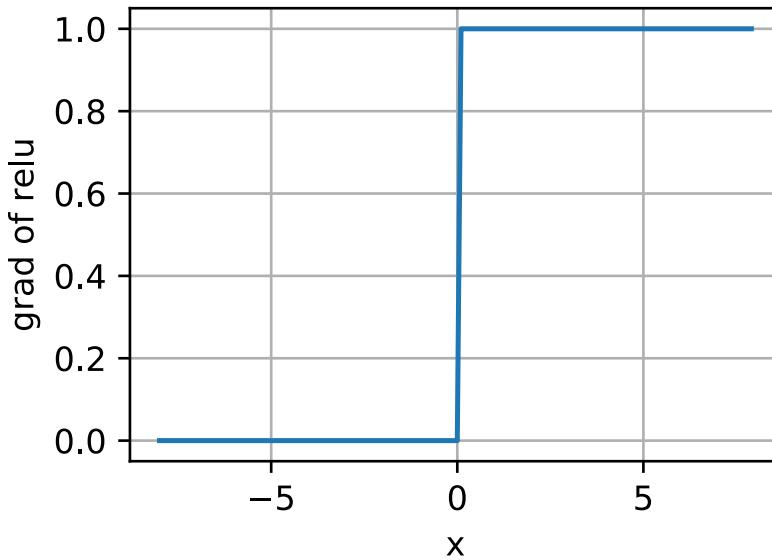
Because it is used so commonly, NDarray supports the `relu` function as a basic native operator. As you can see, the activation function is piece-wise linear.

```
x = nd.arange(-8.0, 8.0, 0.1)
x.attach_grad()
with autograd.record():
    y = x.relu()
d2l.set_figsize((4, 2.5))
d2l.plot(x, y, 'x', 'relu(x)')
```



When the input is negative, the derivative of ReLU function is 0 and when the input is positive, the derivative of ReLU function is 1. Note that the ReLU function is not differentiable when the input takes value precisely equal to 0. In these cases, we go with the left-hand-side (LHS) derivative and say that the derivative is 0 when the input is 0. We can get away with this because the input may never actually be zero. There's an old adage that if subtle boundary conditions matter, we are probably doing (*real*) mathematics, not engineering. That conventional wisdom may apply here. See the derivative of the ReLU function plotted below.

```
y.backward()
d2l.plot(x, x.grad, 'x', 'grad of relu')
```



Note that there are many variants to the ReLU function, such as the parameterized ReLU (pReLU) of He et al., 2015<sup>68</sup>. This variation adds a linear term to the ReLU, so some information still gets through, even

<sup>68</sup> <https://arxiv.org/abs/1502.01852>

when the argument is negative.

$$\text{pReLU}(x) = \max(0, x) + \alpha \min(0, x) \quad (6.1.7)$$

The reason for using the ReLU is that its derivatives are particularly well behaved - either they vanish or they just let the argument through. This makes optimization better behaved and it reduces the issue of the vanishing gradient problem (more on this later).

### Sigmoid Function

The sigmoid function transforms its inputs which take values in  $\mathbb{R}$  to the interval  $(0, 1)$ . For that reason, the sigmoid is often called a *squashing* function: it squashes any input in the range  $(-\infty, \infty)$  to some value in the range  $(0, 1)$ .

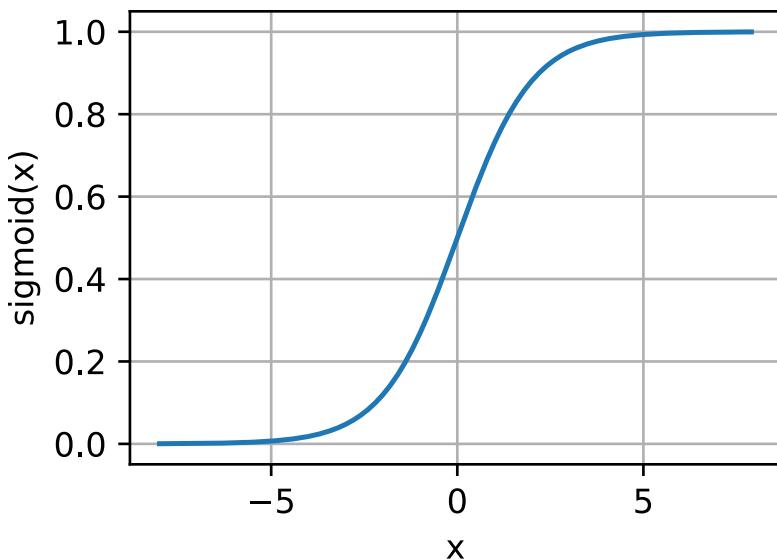
$$\text{sigmoid}(x) = \frac{1}{1 + \exp(-x)}. \quad (6.1.8)$$

In the earliest neural networks, scientists were interested in modeling biological neurons which either *fire* or *don't fire*. Thus the pioneers of this field, going all the way back to McCulloch and Pitts in the 1940s, were focused on thresholding units. A thresholding function takes either value 0 (if the input is below the threshold) or value 1 (if the input exceeds the threshold)

When attention shifted to gradient based learning, the sigmoid function was a natural choice because it is a smooth, differentiable approximation to a thresholding unit. Sigmoids are still common as activation functions on the output units, when we want to interpret the outputs as probabilities for binary classification problems (you can think of the sigmoid as a special case of the softmax) but the sigmoid has mostly been replaced by the simpler and easier to train ReLU for most use in hidden layers. In the “Recurrent Neural Network” chapter, we will describe how sigmoid units can be used to control the flow of information in a neural network thanks to its capacity to transform the value range between 0 and 1.

See the sigmoid function plotted below. When the input is close to 0, the sigmoid function approaches a linear transformation.

```
with autograd.record():
    y = x.sigmoid()
d2l.plot(x, y, 'x', 'sigmoid(x)')
```

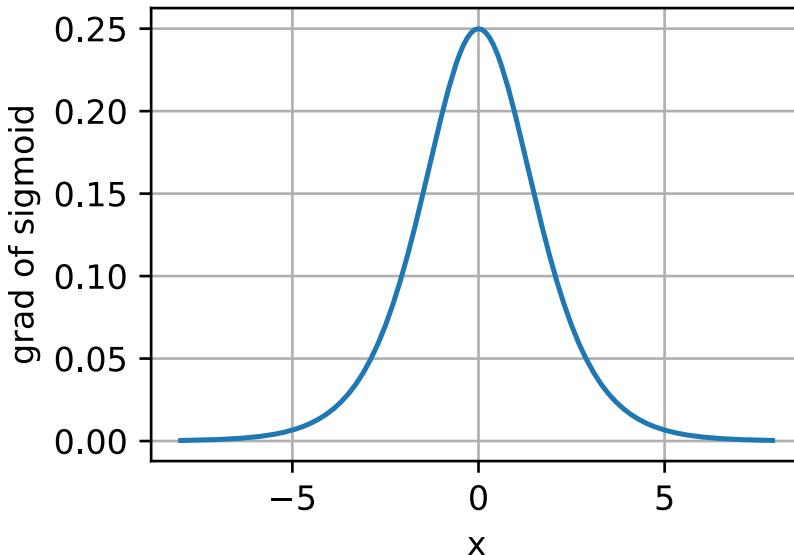


The derivative of sigmoid function is given by the following equation:

$$\frac{d}{dx} \text{sigmoid}(x) = \frac{\exp(-x)}{(1 + \exp(-x))^2} = \text{sigmoid}(x)(1 - \text{sigmoid}(x)). \quad (6.1.9)$$

The derivative of sigmoid function is plotted below. Note that when the input is 0, the derivative of the sigmoid function reaches a maximum of 0.25. As the input diverges from 0 in either direction, the derivative approaches 0.

```
y.backward()
d2l.plot(x, x.grad, 'x', 'grad of sigmoid')
```



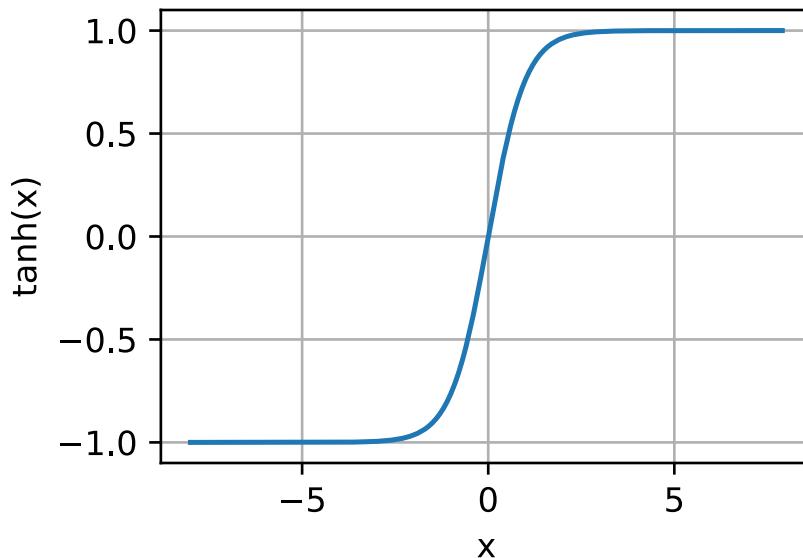
### Tanh Function

Like the sigmoid function, the tanh (Hyperbolic Tangent) function also squashes its inputs, transforms them into elements on the interval between -1 and 1:

$$\tanh(x) = \frac{1 - \exp(-2x)}{1 + \exp(-2x)}. \quad (6.1.10)$$

We plot the tanh function blow. Note that as the input nears 0, the tanh function approaches a linear transformation. Although the shape of the function is similar to the sigmoid function, the tanh function exhibits point symmetry about the origin of the coordinate system.

```
with autograd.record():
    y = x.tanh()
d2l.plot(x, y, 'x', 'tanh(x)')
```

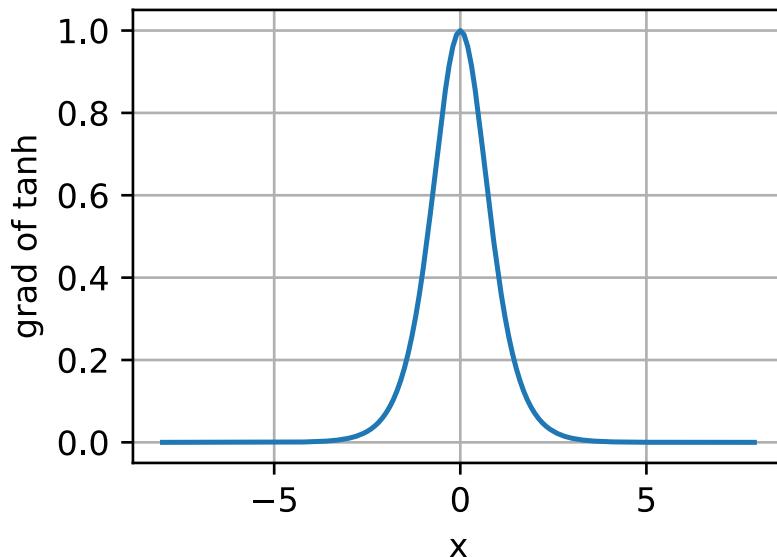


The derivative of the Tanh function is:

$$\frac{d}{dx} \tanh(x) = 1 - \tanh^2(x). \quad (6.1.11)$$

The derivative of tanh function is plotted below. As the input nears 0, the derivative of the tanh function approaches a maximum of 1. And as we saw with the sigmoid function, as the input moves away from 0 in either direction, the derivative of the tanh function approaches 0.

```
y.backward()
d2l.plot(x, x.grad, 'x', 'grad of tanh')
```



In summary, we now know how to incorporate nonlinearities to build expressive multilayer neural network architectures. As a side note, your knowledge now already puts you in command of the state of the art in deep learning, circa 1990. In fact, you have an advantage over anyone working the 1990s, because you can leverage powerful open-source deep learning frameworks to build models rapidly, using only a few lines of

code. Previously, getting these nets training required researchers to code up thousands of lines of C and Fortran.

### 6.1.3 Summary

- The multilayer perceptron adds one or multiple fully-connected hidden layers between the output and input layers and transforms the output of the hidden layer via an activation function.
- Commonly-used activation functions include the ReLU function, the sigmoid function, and the tanh function.

### 6.1.4 Exercises

1. Compute the derivative of the tanh and the pReLU activation function.
2. Show that a multilayer perceptron using only ReLU (or pReLU) constructs a continuous piecewise linear function.
3. Show that  $\tanh(x) + 1 = 2\text{sigmoid}(2x)$ .
4. Assume we have a multilayer perceptron *without* nonlinearities between the layers. In particular, assume that we have  $d$  input dimensions,  $d$  output dimensions and that one of the layers had only  $d/2$  dimensions. Show that this network is less expressive (powerful) than a single layer perceptron.
5. Assume that we have a nonlinearity that applies to one minibatch at a time. What kinds of problems do you expect this to cause?

### 6.1.5 Scan the QR Code to Discuss<sup>69</sup>



## 6.2 Implementation of Multilayer Perceptron from Scratch

Now that we know how multilayer perceptrons (MLPs) work in theory, let's implement them. First, we import the required packages.

```
import d2l
from mxnet import nd, gluon
```

To compare against the results we previously achieved with vanilla softmax regression, we continue to use the Fashion-MNIST image classification dataset.

```
batch_size = 256
train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size)
```

<sup>69</sup> <https://discuss.mxnet.io/t/2338>

## 6.2.1 Initialize Model Parameters

Recall that this dataset contains 10 classes and that each image consists of a  $28 \times 28 = 784$  grid of pixel values. Since we'll be discarding the spatial structure (for now), we can just think of this as a classification dataset with 784 input features and 10 classes. In particular we will implement our MLP with one hidden layer and 256 hidden units. Note that we can regard both of these choices as *hyperparameters* that could be set based on performance on validation data. Typically, we'll choose layer widths as powers of 2 to make everything align nicely in memory.

Again, we will allocate several NDArrays to represent our parameters. Note that we now have one weight matrix and one bias vector *per layer*. As always, we must call `attach_grad` to allocate memory for the gradients with respect to these parameters.

```
num_inputs, num_outputs, num_hiddens = 784, 10, 256

W1 = nd.random.normal(scale=0.01, shape=(num_inputs, num_hiddens))
b1 = nd.zeros(num_hiddens)
W2 = nd.random.normal(scale=0.01, shape=(num_hiddens, num_outputs))
b2 = nd.zeros(num_outputs)
params = [W1, b1, W2, b2]

for param in params:
    param.attach_grad()
```

## 6.2.2 Activation Function

To make sure we know how everything works, we will use the `maximum` function to implement ReLU ourselves, instead of invoking `nd.relu` directly.

```
def relu(X):
    return nd.maximum(X, 0)
```

## 6.2.3 The model

As in softmax regression, we will `reshape` each 2D image into a flat vector of length `num_inputs`. Finally, we can implement our model with just a few lines of code.

```
def net(X):
    X = X.reshape((-1, num_inputs))
    H = relu(nd.dot(X, W1) + b1)
    return nd.dot(H, W2) + b2
```

## 6.2.4 The Loss Function

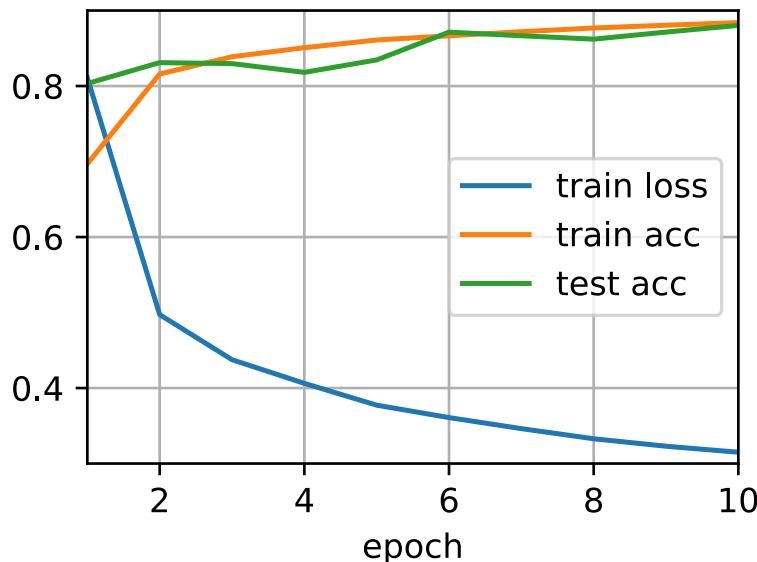
For better numerical stability and because we already know how to implement softmax regression completely from scratch in [Section 5.6](#), we will use Gluon's integrated function for calculating the softmax and cross-entropy loss. Recall that we discussed some of these intricacies in [Section 6.1](#). We encourage the interested reader to examining the source code for `mxnet.gluon.loss.SoftmaxCrossEntropyLoss` for more details.

```
loss = gluon.loss.SoftmaxCrossEntropyLoss()
```

### 6.2.5 Training

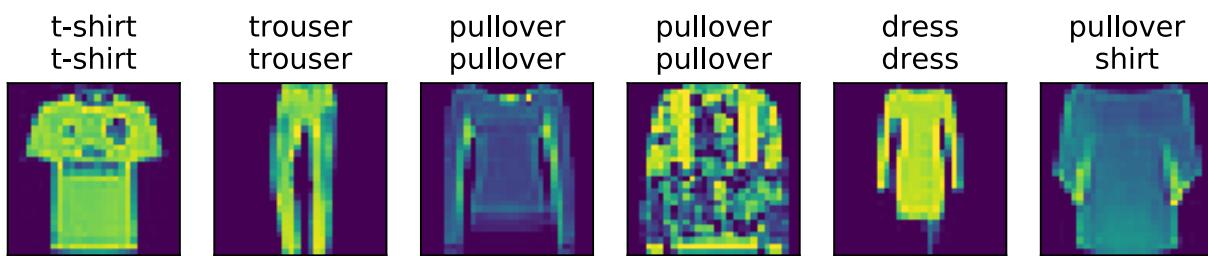
Steps for training the MLP are no different than for softmax regression. In the d2l package, we directly call the `train_ch3` function, whose implementation was introduced in [Section 5.6](#). We set the number of epochs to 10 and the learning rate to 0.5.

```
num_epochs, lr = 10, 0.5
d2l.train_ch3(net, train_iter, test_iter, loss, num_epochs,
              lambda batch_size: d2l.sgd(params, lr, batch_size))
```



To see how well we did, let's apply the model to some test data. If you're interested, compare the result to corresponding linear model in [Section 5.6](#).

```
d2l.predict_ch3(net, test_iter)
```



This looks a bit better than our previous result, a good sign that we're on the right path.

### 6.2.6 Summary

We saw that implementing a simple MLP is easy, even when done manually. That said, with a large number of layers, this can get messy (e.g. naming and keeping track of the model parameters, etc).

## 6.2.7 Exercises

1. Change the value of the hyper-parameter `num_hiddens` in order to see how this hyperparameter influences your results.
2. Try adding a new hidden layer to see how it affects the results.
3. How does changing the learning rate change the result?
4. What is the best result you can get by optimizing over all the parameters (learning rate, iterations, number of hidden layers, number of hidden units per layer)?

## 6.2.8 Scan the QR Code to Discuss<sup>70</sup>



## 6.3 Concise Implementation of Multilayer Perceptron

Now that we learned how multilayer perceptrons (MLPs) work in theory, let's implement them. We begin, as always, by importing modules.

```
import d2l  
from mxnet import gluon, init  
from mxnet.gluon import nn
```

### 6.3.1 The Model

The only difference from our softmax regression implementation is that we add two `Dense` (fully-connected) layers instead of one. The first is our hidden layer, which has 256 hidden units and uses the ReLU activation function.

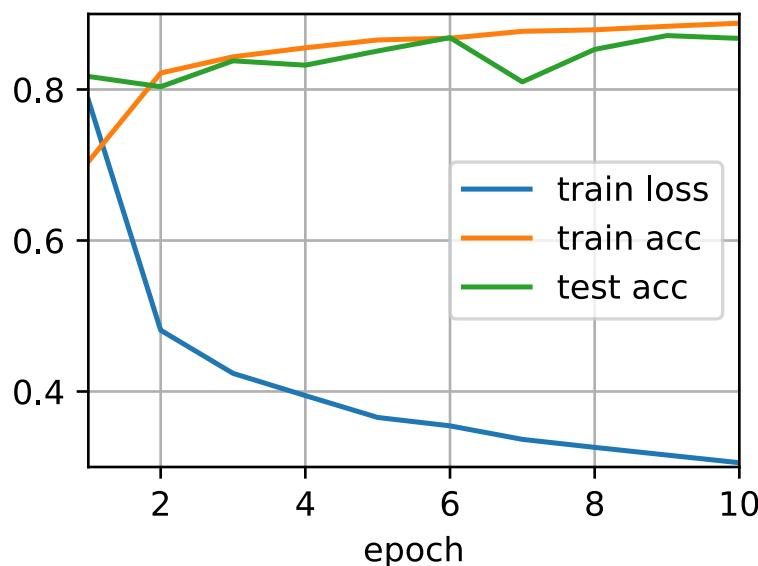
```
net = nn.Sequential()  
net.add(nn.Dense(256, activation='relu'),  
       nn.Dense(10))  
net.initialize(init.Normal(sigma=0.01))
```

Again, note that as always, Gluon automatically infers the missing input dimensions to each layer.

Training the model follows the exact same steps as in our softmax regression implementation.

```
batch_size, num_epochs = 256, 10  
train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size)  
loss = gluon.loss.SoftmaxCrossEntropyLoss()  
trainer = gluon.Trainer(net.collect_params(), 'sgd', {'learning_rate': 0.5})  
d2l.train_ch3(net, train_iter, test_iter, loss, num_epochs, trainer)
```

<sup>70</sup> <https://discuss.mxnet.io/t/2339>



### 6.3.2 Exercises

1. Try adding a few more hidden layers to see how the result changes.
2. Try out different activation functions. Which ones work best?
3. Try out different initializations of the weights.

### 6.3.3 Scan the QR Code to Discuss<sup>71</sup>



## 6.4 Model Selection, Underfitting and Overfitting

As machine learning scientists, our goal is to discover general patterns. Say, for example, that we wish to learn the pattern that associates genetic markers with the development of dementia in adulthood. It's easy enough to memorize our training set. Each person's genes uniquely identify them, not just among people represented in our dataset, but among all people on earth!

Given the genetic markers representing some person, we don't want our model to simply recognize "oh, that's Bob", and then output the classification, say among  $\{\text{dementia}, \text{mild cognitive impairment}, \text{healthy}\}$ , that corresponds to Bob. Rather, our goal is to discover patterns that capture regularities in the underlying population from which our training set was drawn. If we are successfully in this endeavor, then we could successfully assess risk even for individuals that we have never encountered before. This problem—how to discover patterns that *generalize*—is the fundamental problem of machine learning.

<sup>71</sup> <https://discuss.mxnet.io/t/2340>

The danger is that when we train models, we access just a small sample of data. The largest public image datasets contain roughly one million images. And more often we have to learn from thousands or tens of thousands. In a large hospital system we might access hundreds of thousands of medical records. With finite samples, we always run the risk that we might discover *apparent* associations that turn out not to hold up when we collect more data.

Let's consider an extreme pathological case. Imagine that you want to learn to predict which people will repay their loans. A lender hires you as a data scientist to investigate, handing over the complete files on 100 applicants, 5 of which defaulted on their loans within 3 years. Realistically, the files might include hundreds of potential features, including income, occupation, credit score, length of employment etc. Moreover, say that they additionally hand over video footage of each applicant's interview with their lending agent.

Now suppose that after featurizing the data into an enormous design matrix, you discover that of the 5 applicants who default, all of them were wearing blue shirts during their interviews, while only 40% of general population wore blue shirts. There's a good chance that if you train a predictive model to predict default, it might rely upon blue-shirt-wearing as an important feature.

Even if in fact defaulters were no more likely to wear blue shirts than people in the general population, there's a  $.4^5 = .01$  probability that we would observe all five defaulters wearing blue shirts. With just 5 positive examples of defaults and hundreds or thousands of features, we would probably find a large number of features that appear to be perfectly predictive of our labor just due to random chance. With an unlimited amount of data, we would expect these *spurious* associations to eventually disappear. But we seldom have that luxury.

The phenomena of fitting our training data more closely than we fit the underlying distribution is called overfitting, and the techniques used to combat overfitting are called regularization. In the previous sections, you might have observed this effect while experimenting with the Fashion-MNIST dataset. If you altered the model structure or the hyper-parameters during the experiment, you might have noticed that with enough nodes, layers, and training epochs, the model can eventually reach perfect accuracy on the training set, even as the accuracy on test data deteriorates.

### 6.4.1 Training Error and Generalization Error

In order to discuss this phenomenon more formally, we need to differentiate between *training error* and *generalization error*. The training error is the error of our model as calculated on the training data set, while generalization error is the expectation of our model's error were we to apply it to an infinite stream of additional data points drawn from the same underlying data distribution as our original sample.

Problems, we can never calculate the generalization error exactly. That's because the imaginary stream of infinite data is an imaginary object. In practice, we must estimate the generalization error by applying our model to an independent test set constituted of a random selection of data points that were withheld from our training set.

The following three thought experiments will help illustrate this situation better. Consider a college student trying to prepare for his final exam. A diligent student will strive to practice well and test her abilities using exams from previous years. Nonetheless, doing well on past exams is no guarantee that she will excel when it matters. For instance, the student might try to prepare by rote learning the answers to the exam questions. This requires the student to memorize many things. She might even remember the answers for past exams perfectly. Another student might prepare by trying to understand the reasons for giving certain answers. In most cases, the latter student will do much better.

Likewise, consider a model that simply uses a lookup table to answer questions. If the set of allowable inputs is discrete and reasonably small, then perhaps after viewing many training examples, this approach would perform well. Still this model has no ability to do better than random guessing when faced with examples that it has never seen before. In reality the input spaces are far too large to memorize the answers corresponding to every conceivable input. For example, consider the black and white  $28 \times 28$  images. If each pixel can take one among 256 gray scale values, then there are  $256^{784}$  possible images. That means that

there are far more low-res grayscale thumbnail-sized images than there are atoms in the universe. Even if we could encounter this data, we could never afford to store the lookup table.

Lastly, consider the problem of trying to classify the outcomes of coin tosses (class 0: heads, class 1: tails) based on some contextual features that might be available. No matter what algorithm we come up with, because the generalization error will always be  $\frac{1}{2}$ . However, for most algorithms, we should expect our training error to be considerably lower, depending on the luck of the draw, even if we didn't have any features! Consider the dataset  $\{0, 1, 1, 1, 0, 1\}$ . Our feature-less would have to fall back on always predicting the *majority class*, which appears from our limited sample to be 1. In this case, the model that always predicts class 1 will incur an error of  $\frac{1}{3}$ , considerably better than our generalization error. As we increase the amount of data, the probability that the fraction of heads will deviate significantly from  $\frac{1}{2}$  diminishes, and our training error would come to match the generalization error.

## Statistical Learning Theory

Since generalization is the fundamental problem in machine learning, you might not be surprised to learn that many mathematicians and theorists have dedicated their lives to developing formal theories to describe this phenomenon. In their [eponymous theorem<sup>72</sup>](#), Glivenko and Cantelli derived the rate at which the training error converges to the generalization error. In a series of seminal papers, Vapnik and Chervonenkis<sup>73</sup> extended this theory to more general classes of functions. This work laid the foundations of [Statistical Learning Theory<sup>74</sup>](#).

In the **standard supervised learning setting**, which we have addressed up until now and will stick throughout most of this book, we assume that both the training data and the test data are drawn *independently* from *identical* distributions (commonly called the i.i.d. assumption). This means that the process that samples our data has no *memory*. The 2nd example drawn and the 3rd drawn are no more correlated than the 2nd and the 2-millionth sample drawn.

Being a good machine learning scientist requires thinking critically, and already you should be poking holes in this assumption, coming up with common cases where the assumption fails. What if we train a mortality risk predictor on data collected from patients at UCSF, and apply it on patients at Massachusetts General Hospital? These distributions are simply not identical. Moreover, draws might be correlated in time. What if we are classifying the topics of Tweets. The news cycle would create temporal dependencies in the topics being discussed violating any assumptions of independence.

Sometimes we can get away with minor violations of the i.i.d. assumption and our models will continue to work remarkably well. After all, nearly every real-world application involves at least some minor violation of the i.i.d. assumption, and yet we have useful tools for face recognition, speech recognition, language translation, etc.

Other violations are sure to cause trouble. Imagine, for example, if we tried to train a face recognition system by training it exclusively on university students and then want to deploy it as a tool for monitoring geriatrics in a nursing home population. This is unlikely to work well since college students tend to look considerably different from the elderly.

In subsequent chapters and volumes, we will discuss problems arising from violations of the i.i.d. assumption. For now, even taking the i.i.d. assumption for granted, understanding generalization is a formidable problem. Moreover, elucidating the precise theoretical foundations that might explain why deep neural networks generalize as well as they do continues to vexes the greatest minds in learning theory.

When we train our models, we attempt searching for a function that fits the training data as well as possible. If the function is so flexible that it can catch on to spurious patterns just as easily as to the true associations, then it might perform *too well* without producing a model that generalizes well to unseen data. This is

<sup>72</sup> [https://en.wikipedia.org/wiki/Glivenko%20%93Cantelli\\_theorem](https://en.wikipedia.org/wiki/Glivenko%20%93Cantelli_theorem)

<sup>73</sup> [https://en.wikipedia.org/wiki/Vapnik%20%93Chervonenkis\\_theory](https://en.wikipedia.org/wiki/Vapnik%20%93Chervonenkis_theory)

<sup>74</sup> [https://en.wikipedia.org/wiki/Statistical\\_learning\\_theory](https://en.wikipedia.org/wiki/Statistical_learning_theory)

precisely what we want to avoid (or at least control). Many of the techniques in deep learning are heuristics and tricks aimed at guarding against overfitting.

### Model Complexity

When we have simple models and abundant data, we expect the generalization error to resemble the training error. When we work with more complex models and fewer examples, we expect the training error to go down but the generalization gap to grow. What precisely constitutes model complexity is a complex matter. Many factors govern whether a model will generalize well. For example a model with more parameters might be considered more complex. A model whose parameters can take a wider range of values might be more complex. Often with neural networks, we think of a model that takes more training steps as more complex, and one subject to *early stopping* as less complex.

It can be difficult to compare the complexity among members of substantially different model classes (say a decision tree versus a neural network). For now, a simple rule of thumb is quite useful: A model that can readily explain arbitrary facts is what statisticians view as complex, whereas one that has only a limited expressive power but still manages to explain the data well is probably closer to the truth. In philosophy, this is closely related to Popper's criterion of *falsifiability*<sup>75</sup> of a scientific theory: a theory is good if it fits data and if there are specific tests which can be used to disprove it. This is important since all statistical estimation is *post hoc*<sup>76</sup>, i.e. we estimate after we observe the facts, hence vulnerable to the associated fallacy. For now, we'll put the philosophy aside and stick to more tangible issues.

In this chapter, to give you some intuition, we'll focus on a few factors that tend to influence the generalizability of a model class:

1. The number of tunable parameters. When the number of tunable parameters, sometimes called the *degrees of freedom*, is large, models tend to be more susceptible to overfitting.
2. The values taken by the parameters. When weights can take a wider range of values, models can be more susceptible to over fitting.
3. The number of training examples. It's trivially easy to overfit a dataset containing only one or two examples even if your model is simple. But overfitting a dataset with millions of examples requires an extremely flexible model.

#### 6.4.2 Model Selection

In machine learning, we usually select our final model after evaluating several candidate models. This process is called model selection. Sometimes the models subject to comparison are fundamentally different in nature (say, decision trees vs linear models). At other times, we are comparing members of the same class of models that have been trained with different hyperparameter settings.

With multilayer perceptrons for example, we may wish to compare models with different numbers of hidden layers, different numbers of hidden units, and various choices of the activation functions applied to each hidden layer. In order to determine the best among our candidate models, we will typically employ a validation set.

#### Validation Data Set

In principle we should not touch our test set until after we have chosen all our hyper-parameters. Were we to use the test data in the model selection process, there's a risk that we might overfit the test data. Then

<sup>75</sup> <https://en.wikipedia.org/wiki/Falsifiability>

<sup>76</sup> [https://en.wikipedia.org/wiki/Post\\_hoc](https://en.wikipedia.org/wiki/Post_hoc)

we would be in serious trouble. If we overfit our training data, there's always the evaluation on test data to keep us honest. But if we overfit the test data, how would we ever know?

Thus, we should never rely on the test data for model selection. And yet we cannot rely solely on the training data for model selection either because we cannot estimate the generalization error on the very data that we use to train the model.

The common practice to address this problem is to split our data three ways, incorporating a *validation set* in addition to the training and test sets.

In practical applications, the picture gets muddier. While ideally we would only touch the test data once, to assess the very best model or to compare a small number of models to each other, real-world test data is seldom discarded after just one use. We can seldom afford a new test set for each round of experiments.

The result is a murky practice where the boundaries between validation and test data are worryingly ambiguous. Unless explicitly stated otherwise, in the experiments in this book we are really working with what should rightly be called training data and validation data, with no true test sets. Therefore, the accuracy reported in each experiment is really the validation accuracy and not a true test set accuracy. The good news is that we don't need too much data in the validation set. The uncertainty in our estimates can be shown to be of the order of  $O(n^{-\frac{1}{2}})$ .

### K-Fold Cross-Validation

When training data is scarce, we might not even be able to afford to hold out enough data to constitute a proper validation set. One popular solution to this problem is to employ *K-fold cross-validation*. Here, the original training data is split into  $K$  non-overlapping subsets. Then model training and validation are executed  $K$  times, each time training on  $K - 1$  subsets and validating on a different subset (the one not used for training in that round). Finally, the training and validation error rates are estimated by averaging over the results from the  $K$  experiments.

#### 6.4.3 Underfitting or Overfitting?

When we compare the training and validation errors, we want to be mindful of two common situations: First, we want to watch out for cases when our training error and validation error are both substantial but there is a little gap between them. If the model is unable to reduce the training error, that could mean that our model is too simple (i.e., insufficiently expressive) to capture the pattern that we are trying to model. Moreover, since the *generalization gap* between our training and validation errors is small, we have reason to believe that we could get away with a more complex model. This phenomenon is known as underfitting.

On the other hand, as we discussed above, we want to watch out for the cases when our training error is significantly lower than our validation error, indicating severe overfitting. Note that overfitting is not always a bad thing. With deep learning especially, it's well known that the best predictive models often perform far better on training data than on holdout data. Ultimately, we usually care more about the validation error than about the gap between the training and validation errors.

Whether we overfit or underfit can depend both on the complexity of our model and the size of the available training datasets, two topics that we discuss below.

### Model Complexity

To illustrate some classical intuition about overfitting and model complexity, we give an example using polynomials. Given training data consisting of a single feature  $x$  and a corresponding real-valued label  $y$ ,

we try to find the polynomial of degree  $d$

$$\hat{y} = \sum_{i=0}^d x^i w_i \quad (6.4.1)$$

to estimate the labels  $y$ . This is just a linear regression problem where our features are given by the powers of  $x$ , the  $w_i$  given the model's weights, and the bias is given by  $w_0$  since  $x^0 = 1$  for all  $x$ . Since this is just a linear regression problem, we can use the squared error as our loss function.

A higher-order polynomial function is more complex than a lower order polynomial function, since the higher-order polynomial has more parameters and the model function's selection range is wider. Fixing the training data set, higher-order polynomial functions should always achieve lower (at worst, equal) training error relative to lower degree polynomials. In fact, whenever the data points each have a distinct value of  $x$ , a polynomial function with degree equal to the number of data points can fit the training set perfectly. We visualize the relationship between polynomial degree and under- vs over-fitting below.

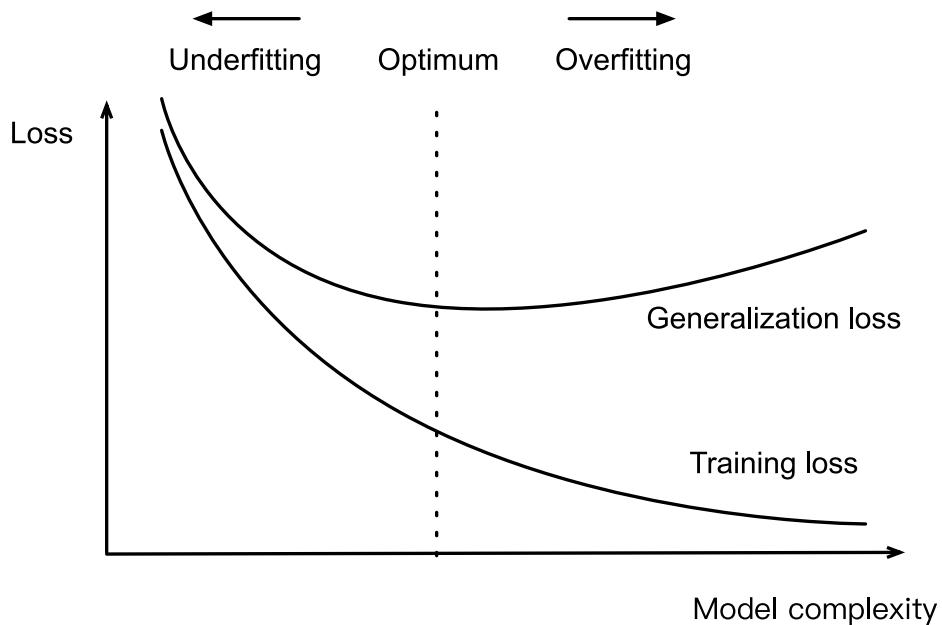


Fig. 6.4.1: Influence of Model Complexity on Underfitting and Overfitting

### Data Set Size

The other big consideration to bear in mind is the dataset size. Fixing our model, the fewer samples we have in the training dataset, the more likely (and more severely) we are to encounter overfitting. As we increase the amount of training data, the generalization error typically decreases. Moreover, in general, more data never hurts. For a fixed task and data *distribution*, there is typically a relationship between model complexity and dataset size. Given more data, we might profitably attempt to fit a more complex model. Absent sufficient data, simpler models may be difficult to beat. For many tasks, deep learning only outperforms linear models when many thousands of training examples are available. In part, the current success of deep learning owes to the current abundance of massive datasets due to internet companies, cheap storage, connected devices, and the broad digitization of the economy.

#### 6.4.4 Polynomial Regression

We can now explore these concepts interactively by fitting polynomials to data. To get started we'll import our usual packages.

```
import d2l
from mxnet import autograd, gluon, nd
from mxnet.gluon import nn
```

##### Generating Data Sets

First we need data. Given  $x$ , we will use the following cubic polynomial to generate the labels on training and test data:

$$y = 5 + 1.2x - 3.4 \frac{x^2}{2!} + 5.6 \frac{x^3}{3!} + \epsilon \text{ where } \epsilon \sim \mathcal{N}(0, 0.1) \quad (6.4.2)$$

The noise term  $\epsilon$  obeys a normal distribution with a mean of 0 and a standard deviation of 0.1. We'll synthesize 100 samples each for the training set and test set.

```
maxdegree = 20 # Maximum degree of the polynomial
n_train, n_test = 100, 100 # Training and test data set sizes
true_w = nd.zeros(maxdegree) # Allocate lots of empty space
true_w[0:4] = nd.array([5, 1.2, -3.4, 5.6])

features = nd.random.normal(shape=(n_train + n_test, 1))
features = nd.random.shuffle(features)
poly_features = nd.power(features, nd.arange(maxdegree).reshape((1, -1)))
poly_features = poly_features / (
    nd.gamma(nd.arange(maxdegree) + 1).reshape((1, -1)))
labels = nd.dot(poly_features, true_w)
labels += nd.random.normal(scale=0.1, shape=labels.shape)
```

For optimization, we typically want to avoid very large values of gradients, losses, etc. This is why the monomials stored in `poly_features` are rescaled from  $x^i$  to  $\frac{1}{i!}x^i$ . It allows us to avoid very large values for large exponents  $i$ . Factorials are implemented in Gluon using the Gamma function, where  $n! = \Gamma(n + 1)$ .

Take a look at the first 2 samples from the generated data set. The value 1 is technically a feature, namely the constant feature corresponding to the bias.

```
features[:2], poly_features[:2], labels[:2]
```

```
([[1.5094751
  [1.9676613]
<NDArray 2x1 @cpu(0)>,
 [[1.0000000e+00 1.5094751e+00 1.1392574e+00 5.7322693e-01 2.1631797e-01
  6.5305315e-02 1.6429458e-02 3.5428370e-03 6.6847802e-04 1.1211676e-04
  1.6923748e-05 2.3223611e-06 2.9212887e-07 3.3920095e-08 3.6572534e-09
  3.6803552e-10 3.4721288e-11 3.0829944e-12 2.5853909e-13 2.0539909e-14]
 [[1.0000000e+00 1.9676613e+00 1.9358451e+00 1.2696959e+00 6.2458295e-01
  2.4579351e-01 8.0606394e-02 2.2658013e-02 5.5729118e-03 1.2184002e-03
  2.3973989e-04 4.2884261e-05 7.0318083e-06 1.0643244e-06 1.4958786e-07
  1.9622549e-08 2.4131586e-09 2.7931044e-10 3.0532687e-11 3.1619987e-12]]
```

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```
<NDArray 2x20 @cpu(0)>,
[6.1804767 7.7595935]
<NDArray 2 @cpu(0)>
```

## Defining, Training and Testing Model

Let first implement a function to evaluate the loss on a given data.

```
# Save to the d2l package.
def evaluate_loss(net, data_iter, loss):
    """Evaluate the loss of a model on the given dataset"""
    metric = d2l.Accumulator(2) # sum_loss, num_examples
    for X, y in data_iter:
        metric.add(loss(net(X), y).sum().asscalar(), y.size)
    return metric[0] / metric[1]
```

Now define the training function.

```
def train(train_features, test_features, train_labels, test_labels,
          num_epochs=1000):
    loss = gluon.loss.L2Loss()
    net = nn.Sequential()
    # Switch off the bias since we already catered for it in the polynomial
    # features
    net.add(nn.Dense(1, use_bias=False))
    net.initialize()
    batch_size = min(10, train_labels.shape[0])
    train_iter = d2l.load_array((train_features, train_labels), batch_size)
    test_iter = d2l.load_array((test_features, test_labels), batch_size,
                               is_train=False)
    trainer = gluon.Trainer(net.collect_params(), 'sgd',
                           {'learning_rate': 0.01})
    animator = d2l.Animator(xlabel='epoch', ylabel='loss', yscale='log',
                            xlim=[1,num_epochs], ylim=[1e-3, 1e2],
                            legend=['train', 'test'])
    for epoch in range(1, num_epochs+1):
        d2l.train_epoch_ch3(net, train_iter, loss, trainer)
        if epoch % 50 == 0:
            animator.add(epoch, (evaluate_loss(net, train_iter, loss),
                                evaluate_loss(net, test_iter, loss)))
    print('weight:', net[0].weight.data().asnumpy())
```

## Third-order Polynomial Function Fitting (Normal)

We will begin by first using a third-order polynomial function with the same order as the data generation function. The results show that this model's training error rate when using the testing data set is low. The trained model parameters are also close to the true values  $w = [5, 1.2, -3.4, 5.6]$ .

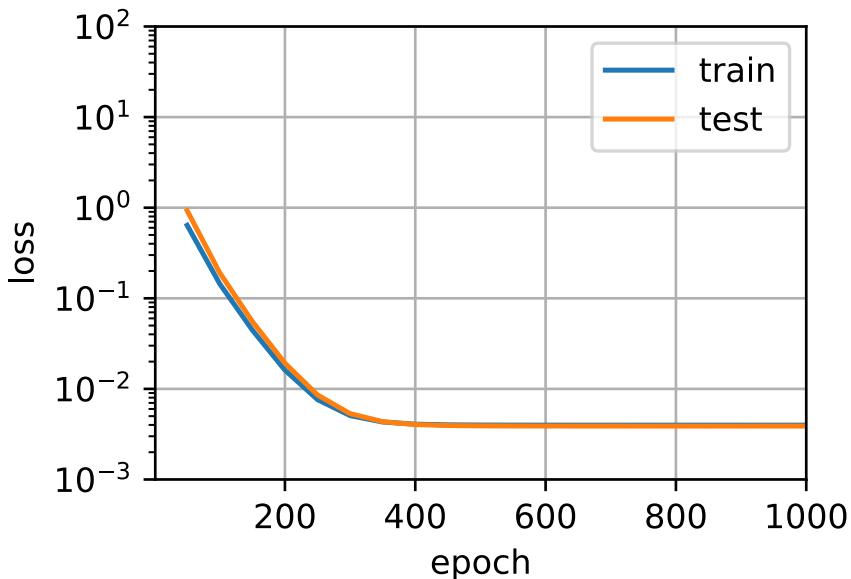
```
# Pick the first four dimensions, i.e. 1, x, x^2, x^3 from the polynomial
# features
```

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```
train(poly_features[:n_train, 0:4], poly_features[n_train:, 0:4],
      labels[:n_train], labels[n_train:])
```

```
weight: [[ 5.016264    1.1760055   -3.418437    5.6421647]]
```

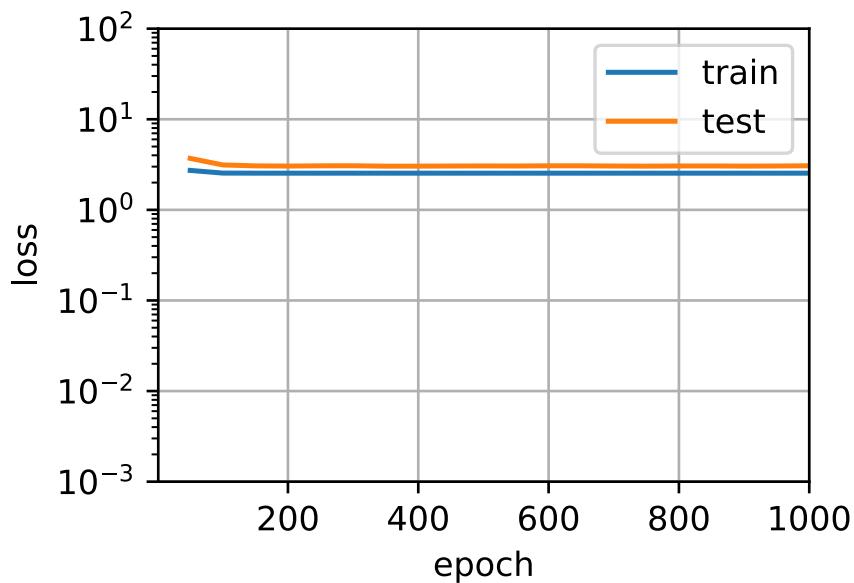


### Linear Function Fitting (Underfitting)

Let's take another look at linear function fitting. After the decline in the early epoch, it becomes difficult to further decrease this model's training error rate. After the last epoch iteration has been completed, the training error rate is still high. When used to fit non-linear patterns (like the third-order polynomial function here) linear models are liable to underfit.

```
# Pick the first four dimensions, i.e. 1, x from the polynomial features
train(poly_features[:n_train, 0:3], poly_features[n_train:, 0:3],
      labels[:n_train], labels[n_train:])
```

```
weight: [[ 4.8976    4.115321   -2.354986]]
```



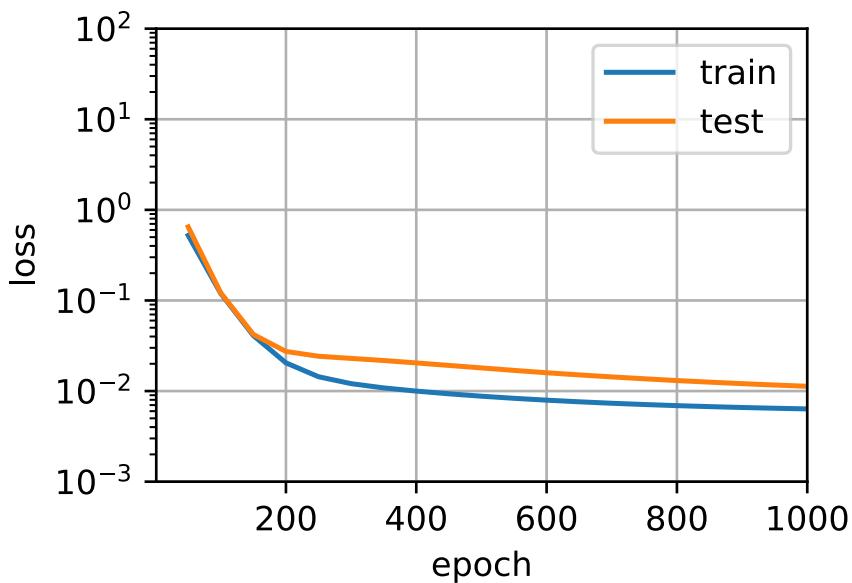
### Insufficient Training (Overfitting)

Now let's try to train the model using a polynomial of too high degree. Here, there is insufficient data to learn that the higher-degree coefficients should have values close to zero. As a result, our overly-complex model is far too susceptible to being influenced by noise in the training data. Of course, our training error will now be low (even lower than if we had the right model!) but our test error will be high.

Try out different model complexities (`n_degree`) and training set sizes (`n_subset`) to gain some intuition of what is happening.

```
n_subset = 100 # Subset of data to train on
n_degree = 20 # Degree of polynomials
train(poly_features[1:n_subset, 0:n_degree],
      poly_features[n_train:, 0:n_degree], labels[1:n_subset],
      labels[n_train:])
```

```
weight: [[ 4.983746   1.3022454  -3.2613719   5.037552  -0.37990612  1.6089656
  0.04346402  0.22759269 -0.03205246  0.03358962 -0.01791902  0.01421152
  0.00740884  0.01047217 -0.06528624  0.02145074  0.06565466  0.02129446
 -0.02506039 -0.00960142]]
```



In later chapters, we will continue to discuss overfitting problems and methods for dealing with them, such as weight decay and dropout.

#### 6.4.5 Summary

- Since the generalization error rate cannot be estimated based on the training error rate, simply minimizing the training error rate will not necessarily mean a reduction in the generalization error rate. Machine learning models need to be careful to safeguard against overfitting such as to minimize the generalization error.
- A validation set can be used for model selection (provided that it isn't used too liberally).
- Underfitting means that the model is not able to reduce the training error rate while overfitting is a result of the model training error rate being much lower than the testing data set rate.
- We should choose an appropriately complex model and avoid using insufficient training samples.

#### 6.4.6 Exercises

1. Can you solve the polynomial regression problem exactly? Hint - use linear algebra.
2. Model selection for polynomials
  - Plot the training error vs. model complexity (degree of the polynomial). What do you observe?
  - Plot the test error in this case.
  - Generate the same graph as a function of the amount of data?
3. What happens if you drop the normalization of the polynomial features  $x^i$  by  $1/i!$ . Can you fix this in some other way?
4. What degree of polynomial do you need to reduce the training error to 0?
5. Can you ever expect to see 0 generalization error?

### 6.4.7 Scan the QR Code to Discuss<sup>77</sup>



## 6.5 Weight Decay

Now that we have characterized the problem of overfitting and motivated the need for capacity control, we can begin discussing some of the popular techniques used to these ends in practice. Recall that we can always mitigate overfitting by going out and collecting more training data, that can be costly and time consuming, typically making it impossible in the short run. For now, let's assume that we have already obtained as much high-quality data as our resources permit and focus on techniques aimed at limiting the capacity of the function classes under consideration.

In our toy example, we saw that we could control the complexity of a polynomial by adjusting its degree. However, most of machine learning does not consist of polynomial curve fitting. And moreover, even when we focus on polynomial regression, when we deal with high-dimensional data, manipulating model capacity by tweaking the degree  $d$  is problematic. To see why, note that for multivariate data we must generalize the concept of polynomials to include *monomials*, which are simply products of powers of variables. For example,  $x_1^2x_2$ , and  $x_3x_5^2$  are both monomials of degree 3. The number of such terms with a given degree  $d$  blows up as a function of the degree  $d$ .

Concretely, for vectors of dimensionality  $D$ , the number of monomials of a given degree  $d$  is  $\binom{D-1+d}{D-1}$ . Hence, a small change in degree, even from say 1 to 2 or 2 to 3 would entail a massive blowup in the complexity of our model. Thus, tweaking the degree is too blunt a hammer. Instead, we need a more fine-grained tool for adjusting function complexity.

### 6.5.1 Squared Norm Regularization

*Weight decay* (commonly called *L2 regularization*), might be the most widely-used technique for regularizing parametric machine learning models. The basic intuition behind weight decay is the notion that among all functions  $f$ , the function  $f = 0$  is the simplest. Intuitively, we can then measure functions by their proximity to zero. But how precisely should we measure the distance between a function and zero? There is no single right answer. In fact, entire branches of mathematics, e.g. in functional analysis and the theory of Banach spaces are devoted to answering this issue.

For our present purposes, a very simple interpretation will suffice: We will consider a linear function  $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$  to be simple if its weight vector is small. We can measure this via  $\|\mathbf{w}\|^2$ . One way of keeping the weight vector small is to add its norm as a penalty term to the problem of minimizing the loss. Thus we replace our original objective, *minimize the prediction error on the training labels*, with new objective, *minimize the sum of the prediction error and the penalty term*. Now, if the weight vector becomes too large, our learning algorithm will find more profit in minimizing the norm  $\|\mathbf{w}\|^2$  versus minimizing the training error. That's exactly what we want. To illustrate things in code, let's revive our previous example from [Section 5.1](#) for linear regression. There, our loss was given by

$$l(\mathbf{w}, b) = \frac{1}{n} \sum_{i=1}^n \frac{1}{2} \left( \mathbf{w}^\top \mathbf{x}^{(i)} + b - y^{(i)} \right)^2. \quad (6.5.1)$$

---

<sup>77</sup> <https://discuss.mxnet.io/t/2341>

Recall that  $\mathbf{x}^{(i)}$  are the observations,  $y^{(i)}$  are labels, and  $(\mathbf{w}, b)$  are the weight and bias parameters respectively. To arrive at a new loss function that penalizes the size of the weight vector, we need to add  $\|\mathbf{w}\|^2$ , but how much should we add? To address this, we need to add a new hyperparameter, that we will call the *regularization constant* and denote by  $\lambda$ :

$$l(\mathbf{w}, b) + \frac{\lambda}{2} \|\mathbf{w}\|^2 \quad (6.5.2)$$

This non-negative parameter  $\lambda \geq 0$  governs the amount of regularization. For  $\lambda = 0$ , we recover our original loss function, whereas for  $\lambda > 0$  we ensure that  $\mathbf{w}$  cannot grow too large. The astute reader might wonder why we are squaring the norm of the weight vector. We do this for two reasons. First, we do it for computational convenience. By squaring the L2 norm, we remove the square root, leaving the sum of squares of each component of the weight vector. This is convenient because it is easy to compute derivatives of a sum of terms (the sum of derivatives equals the derivative of the sum).

Moreover, you might ask, why the L2 norm in the first place and not the L1 norm, or some other distance function. In fact, several other choices are valid and are popular throughout statistics. While L2-regularized linear models constitute the classic *ridge regression* algorithm L1-regularized linear regression is a similarly fundamental model in statistics popularly known as *lasso regression*.

One mathematical reason for working with the L2 norm and not some other norm, is that it penalizes large components of the weight vector much more than it penalizes small ones. This encourages our learning algorithm to discover models which distribute their weight across a larger number of features, which might make them more robust in practice since they do not depend precariously on a single feature. The stochastic gradient descent updates for L2-regularized regression are as follows:

$$\mathbf{w} \leftarrow \left(1 - \frac{\eta\lambda}{|\mathcal{B}|}\right) \mathbf{w} - \frac{\eta}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \mathbf{x}^{(i)} \left(\mathbf{w}^\top \mathbf{x}^{(i)} + b - y^{(i)}\right), \quad (6.5.3)$$

As before, we update  $\mathbf{w}$  based on the amount by which our estimate differs from the observation. However, we also shrink the size of  $\mathbf{w}$  towards 0. That's why the method is sometimes called "weight decay": because the penalty term literally causes our optimization algorithm to *decay* the magnitude of the weight at each step of training. This is more convenient than having to pick the number of parameters as we did for polynomials. In particular, we now have a continuous mechanism for adjusting the complexity of  $f$ . Small values of  $\lambda$  correspond to unconstrained  $\mathbf{w}$ , whereas large values of  $\lambda$  constrain  $\mathbf{w}$  considerably. Since we don't want to have large bias terms either, we often add  $b^2$  as a penalty, too.

## 6.5.2 High-dimensional Linear Regression

For high-dimensional regression it is difficult to pick the 'right' dimensions to omit. Weight-decay regularization is a much more convenient alternative. We will illustrate this below. First, we will generate some synthetic data as before

$$y = 0.05 + \sum_{i=1}^d 0.01x_i + \epsilon \text{ where } \epsilon \sim \mathcal{N}(0, 0.01) \quad (6.5.4)$$

representing our label as a linear function of our inputs, corrupted by Gaussian noise with zero mean and variance 0.01. To observe the effects of overfitting more easily, we can make our problem high-dimensional, setting the data dimension to  $d = 200$  and working with a relatively small number of training examples—here we'll set the sample size to 20:

```
%matplotlib inline
import d2l
from mxnet import autograd, gluon, init, nd
```

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```
from mxnet.gluon import nn

n_train, n_test, num_inputs, batch_size = 20, 100, 200, 1
true_w, true_b = nd.ones((num_inputs, 1)) * 0.01, 0.05
train_data = d2l.synthetic_data(true_w, true_b, n_train)
train_iter = d2l.load_array(train_data, batch_size)
test_data = d2l.synthetic_data(true_w, true_b, n_test)
test_iter = d2l.load_array(test_data, batch_size, is_train=False)
```

### 6.5.3 Implementation from Scratch

Next, we will show how to implement weight decay from scratch. All we have to do here is to add the squared  $\ell_2$  penalty as an additional loss term added to the original target function. The squared norm penalty derives its name from the fact that we are adding the second power  $\sum_i w_i^2$ . The  $\ell_2$  is just one among an infinite class of norms call p-norms, many of which you might encounter in the future. In general, for some number  $p$ , the  $\ell_p$  norm is defined as

$$\|\mathbf{w}\|_p^p := \sum_{i=1}^d |w_i|^p \quad (6.5.5)$$

#### Initialize Model Parameters

First, we'll define a function to randomly initialize our model parameters and run `attach_grad` on each to allocate memory for the gradients we will calculate.

```
def init_params():
    w = nd.random.normal(scale=1, shape=(num_inputs, 1))
    b = nd.zeros(shape=(1,))
    w.attach_grad()
    b.attach_grad()
    return [w, b]
```

#### Define $\ell_2$ Norm Penalty

Perhaps the most convenient way to implement this penalty is to square all terms in place and summ them up. We divide by 2 by convention (when we take the derivative of a quadratic function, the 2 and 1/2 cancel out, ensuring that the expression for the update looks nice and simple).

```
def l2_penalty(w):
    return (w**2).sum() / 2
```

#### Define Training and Testing

The following code defines how to train and test the model separately on the training data set and the test data set. Unlike the previous sections, here, the  $\ell_2$  norm penalty term is added when calculating the final loss function. The linear network and the squared loss haven't changed since the previous chapter, so we'll just import them via `d2l.linreg` and `d2l.squared_loss` to reduce clutter.

```

def train(lambd):
    w, b = init_params()
    net, loss = lambda X: d2l.linreg(X, w, b), d2l.squared_loss
    num_epochs, lr = 100, 0.003
    animator = d2l.Animator(xlabel='epochs', ylabel='loss', yscale='log',
                             xlim=[1, num_epochs], legend=['train', 'test'])
    for epoch in range(1, num_epochs+1):
        for X, y in train_iter:
            with autograd.record():
                # The L2 norm penalty term has been added
                l = loss(net(X), y) + lambd * l2_penalty(w)
            l.backward()
            d2l.sgd([w, b], lr, batch_size)
        if epoch % 5 == 0:
            animator.add(epoch+1, (d2l.evaluate_loss(net, train_iter, loss),
                                  d2l.evaluate_loss(net, test_iter, loss)))
    print('l2 norm of w:', w.norm().asscalar())

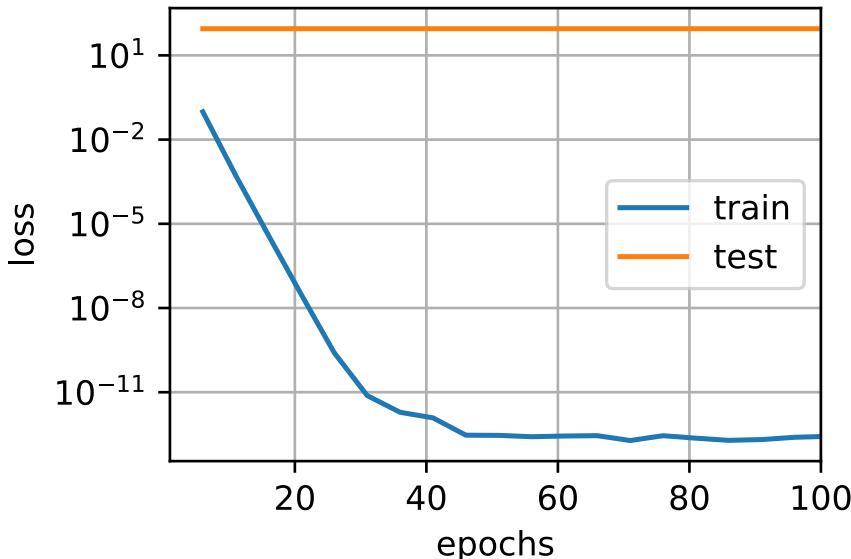
```

### Training without Regularization

Next, let's train and test the high-dimensional linear regression model. When `lambd = 0` we do not use weight decay. As a result, while the training error decreases, the test error does not. This is a perfect example of overfitting.

```
train(lambd=0)
```

```
l2 norm of w: 13.949476
```



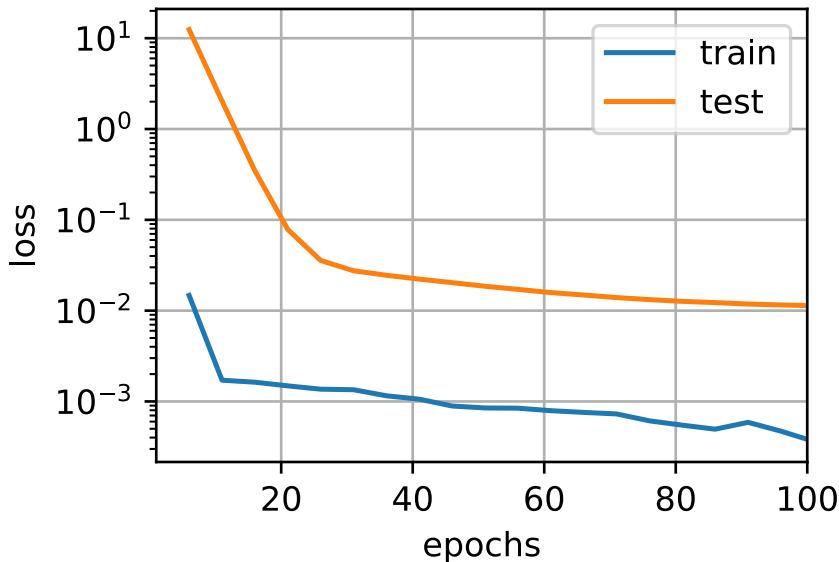
### Using Weight Decay

The example below shows that even though the training error increased, the error on the test set decreased. This is precisely the improvement that we expect from using weight decay. While not perfect, overfitting

has been mitigated to some extent. In addition, the  $\ell_2$  norm of the weight  $\mathbf{w}$  is smaller than without using weight decay.

```
train(lambd=3)
```

```
l2 norm of w: 0.044366416
```



#### 6.5.4 Concise Implementation

Because weight decay is ubiquitous in neural network optimization, Gluon makes it especially convenient, integrating weight decay into the optimization algorithm itself for easy use in combination with any loss function. Moreover, this integration serves a computational benefit, allowing implementation tricks to add weight decay to the algorithm, without any additional computational overhead. Since the weight decay portion of the update depends only on the current value of each parameter, and the optimizer must touch each parameter once anyway.

In the following code, we specify the weight decay hyper-parameter directly through the `wd` parameter when instantiating our `Trainer`. By default, Gluon decays both weights and biases simultaneously. Note that we can have *different* optimizers for different sets of parameters. For instance, we can have one `Trainer` with weight decay for the weights  $\mathbf{w}$  and another without weight decay to take care of the bias  $b$ .

```
def train_gluon(wd):
    net = nn.Sequential()
    net.add(nn.Dense(1))
    net.initialize(init.Normal(sigma=1))
    loss = gluon.loss.L2Loss()
    num_epochs, lr = 100, 0.003
    # The weight parameter has been decayed. Weight names generally end with
    # "weight".
    trainer_w = gluon.Trainer(net.collect_params('.*weight'), 'sgd',
                               {'learning_rate': lr, 'wd': wd})
    # The bias parameter has not decayed. Bias names generally end with "bias"
    trainer_b = gluon.Trainer(net.collect_params('.*bias'), 'sgd',
```

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```

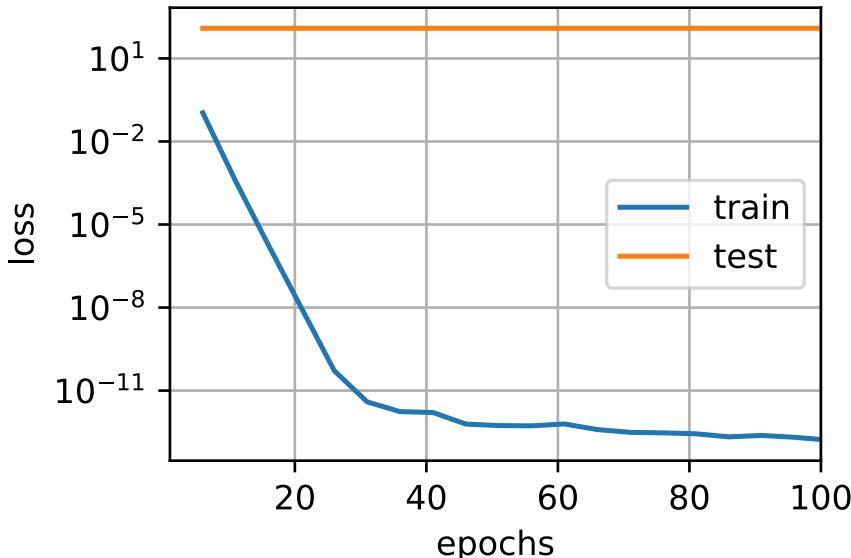
        {'learning_rate': lr})
animator = d2l.Animator(xlabel='epochs', ylabel='loss',
                         xlim=[1, num_epochs], legend=['train', 'test'])
for epoch in range(1, num_epochs+1):
    for X, y in train_iter:
        with autograd.record():
            l = loss(net(X), y)
            l.backward()
            # Call the step function on each of the two Trainer instances to
            # update the weight and bias separately
            trainer_w.step(batch_size)
            trainer_b.step(batch_size)
    if epoch % 5 == 0:
        animator.add(epoch+1, (d2l.evaluate_loss(net, train_iter, loss),
                               d2l.evaluate_loss(net, test_iter, loss)))
print('L2 norm of w:', net[0].weight.data().norm().asscalar())

```

The plots look just the same as when we implemented weight decay from scratch but they run a bit faster and are easier to implement, a benefit that will become more pronounced for large problems.

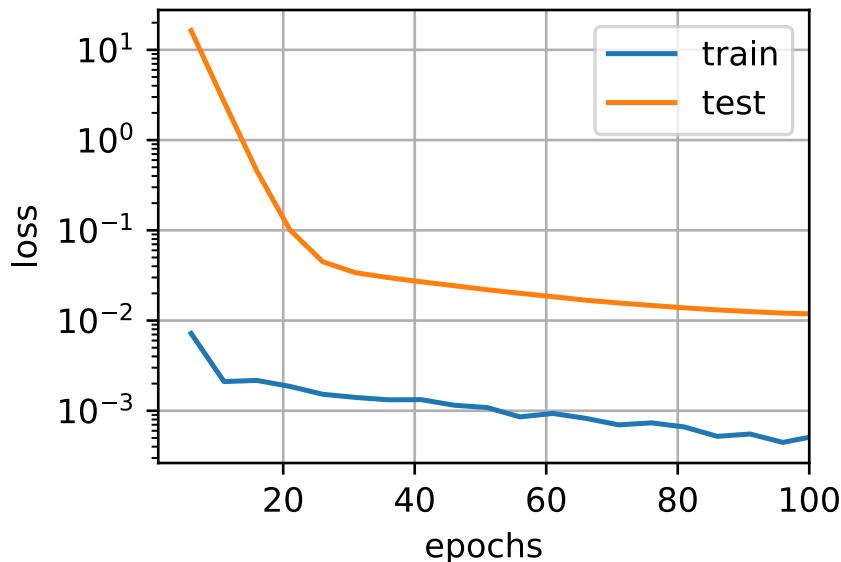
```
train_gluon(0)
```

```
L2 norm of w: 13.989462
```



```
train_gluon(3)
```

```
L2 norm of w: 0.0452111
```



So far, we only touched upon one notion of what constitutes a simple *linear* function. For nonlinear functions, what constitutes *simplicity* can be a far more complex question. For instance, there exist [Reproducing Kernel Hilbert Spaces \(RKHS\)](#)<sup>78</sup> which allow one to use many of the tools introduced for linear functions in a nonlinear context. Unfortunately, RKHS-based algorithms do not always scale well to massive amounts of data. For the purposes of this book, we limit ourselves to simply summing over the weights for different layers, e.g. via  $\sum_l \|\mathbf{w}_l\|^2$ , which is equivalent to weight decay applied to all layers.

### 6.5.5 Summary

- Regularization is a common method for dealing with overfitting. It adds a penalty term to the loss function on the training set to reduce the complexity of the learned model.
- One particular choice for keeping the model simple is weight decay using an  $\ell_2$  penalty. This leads to weight decay in the update steps of the learning algorithm.
- Gluon provides automatic weight decay functionality in the optimizer by setting the hyperparameter `wd`.
- You can have different optimizers within the same training loop, e.g. for different sets of parameters.

### 6.5.6 Exercises

1. Experiment with the value of  $\lambda$  in the estimation problem in this page. Plot training and test accuracy as a function of  $\lambda$ . What do you observe?
2. Use a validation set to find the optimal value of  $\lambda$ . Is it really the optimal value? Does this matter?
3. What would the update equations look like if instead of  $\|\mathbf{w}\|^2$  we used  $\sum_i |w_i|$  as our penalty of choice (this is called  $\ell_1$  regularization).
4. We know that  $\|\mathbf{w}\|^2 = \mathbf{w}^\top \mathbf{w}$ . Can you find a similar equation for matrices (mathematicians call this the [Frobenius norm](#)<sup>79</sup>)?

<sup>78</sup> [https://en.wikipedia.org/wiki/Reproducing\\_kernel\\_Hilbert\\_space](https://en.wikipedia.org/wiki/Reproducing_kernel_Hilbert_space)

<sup>79</sup> [https://en.wikipedia.org/wiki/Matrix\\_norm#Frobenius\\_norm](https://en.wikipedia.org/wiki/Matrix_norm#Frobenius_norm)

5. Review the relationship between training error and generalization error. In addition to weight decay, increased training, and the use of a model of suitable complexity, what other ways can you think of to deal with overfitting?
6. In Bayesian statistics we use the product of prior and likelihood to arrive at a posterior via  $p(w|x) \propto p(x|w)p(w)$ . How can you identify  $p(w)$  with regularization?

### 6.5.7 Scan the QR Code to Discuss<sup>80</sup>



## 6.6 Dropout

Just now, we introduced the classical approach of regularizing statistical models by penalizing the  $\ell_2$  norm of the weights. In probabilistic terms, we could justify this technique by arguing that we have assumed a prior belief that weights take values from a Gaussian distribution with mean 0. More intuitively, we might argue that we encouraged the model to spread out its weights among many features and rather than depending too much on a small number of potentially spurious associations.

### 6.6.1 Overfitting Revisited

Given many more features than examples, linear models can overfit. But when there are many more examples than features, we can generally count on linear models not to overfit. Unfortunately, the reliability with which linear models generalize comes at a cost: Linear models can't take into account interactions among features. For every feature, a linear model must assign either a positive or a negative weight. They lack the flexibility to account for context.

In more formal texts, you'll see this fundamental tension between generalizability and flexibility discussed as the *bias-variance tradeoff*. Linear models have high bias (they can only represent a small class of functions), but low variance (they give similar results across different random samples of the data).

Deep neural networks take us to the opposite end of the bias-variance spectrum. Neural networks are so flexible because they aren't confined to looking at each feature individually. Instead, they can learn interactions among groups of features. For example, they might infer that "Nigeria" and "Western Union" appearing together in an email indicates spam but that "Nigeria" without "Western Union" does not.

Even when we only have a small number of features, deep neural networks are capable of overfitting. In 2017, a group of researchers presented a now well-known demonstration of the incredible flexibility of neural networks. They presented a neural network with randomly-labeled images (there was no true pattern linking the inputs to the outputs) and found that the neural network, optimized by SGD, could label every image in the training set perfectly.

Consider what this means. If the labels are assigned uniformly at random and there are 10 classes, then no classifier can get better than 10% accuracy on holdout data. Yet even in these situations, when there is no true pattern to be learned, neural networks can perfectly fit the training labels.

<sup>80</sup> <https://discuss.mxnet.io/t/2342>

## 6.6.2 Robustness through Perturbations

Let's think briefly about what we expect from a good statistical model. We want it to do well on unseen test data. One way we can accomplish this is by asking what constitutes a 'simple' model? Simplicity can come in the form of a small number of dimensions, which is what we did when discussing fitting a model with monomial basis functions. Simplicity can also come in the form of a small norm for the basis functions. This led us to weight decay ( $\ell_2$  regularization). Yet a third notion of simplicity that we can impose is that the function should be robust under small changes in the input. For instance, when we classify images, we would expect that adding some random noise to the pixels should be mostly harmless.

In 1995, Christopher Bishop formalized a form of this idea when he proved that training with input noise is equivalent to Tikhonov regularization [2]. In other words, he drew a clear mathematical connection between the requirement that a function be smooth (and thus simple), as we discussed in the section on weight decay, with and the requirement that it be resilient to perturbations in the input.

Then in 2014, Srivastava et al. [55] developed a clever idea for how to apply Bishop's idea to the *internal* layers of the network, too. Namely they proposed to inject noise into each layer of the network before calculating the subsequent layer during training. They realized that when training deep network with many layers, enforcing smoothness just on the input-output mapping misses out on what is happening internally in the network. Their proposed idea is called *dropout*, and it is now a standard technique that is widely used for training neural networks. Throughout training, on each iteration, dropout regularization consists simply of zeroing out some fraction (typically 50%) of the nodes in each layer before calculating the subsequent layer.

The key challenge then is how to inject this noise without introducing undue statistical *bias*. In other words, we want to perturb the inputs to each layer during training in such a way that the expected value of the layer is equal to the value it would have taken had we not introduced any noise at all.

In Bishop's case, when we are adding Gaussian noise to a linear model, this is simple: At each training iteration, just add noise sampled from a distribution with mean zero  $\epsilon \sim \mathcal{N}(0, \sigma^2)$  to the input  $\mathbf{x}$ , yielding a perturbed point  $\mathbf{x}' = \mathbf{x} + \epsilon$ . In expectation,  $\mathbf{E}[\mathbf{x}'] = \mathbf{x}$ .

In the case of dropout regularization, one can debias each layer by normalizing by the fraction of nodes that were not dropped out. In other words, dropout with drop probability  $p$  is applied as follows:

$$h' = \begin{cases} 0 & \text{with probability } p \\ \frac{h}{1-p} & \text{otherwise} \end{cases} \quad (6.6.1)$$

By design, the expectation remains unchanged, i.e.,  $\mathbf{E}[h'] = h$ . Intermediate activations  $h$  are replaced by a random variable  $h'$  with matching expectation. The name 'dropout' arises from the notion that some neurons 'drop out' of the computation for the purpose of computing the final result. During training, we replace intermediate activations with random variables.

## 6.6.3 Dropout in Practice

Recall the multilayer perceptron (Section 6.1) with a hidden layer and 5 hidden units. Its architecture is given by

$$\begin{aligned} h &= \sigma(W_1x + b_1) \\ o &= W_2h + b_2 \\ \hat{y} &= \text{softmax}(o) \end{aligned} \quad (6.6.2)$$

When we apply dropout to the hidden layer, we are essentially removing each hidden unit with probability  $p$ , (i.e., setting their output to 0). We can view the result as a network containing only a subset of the original neurons. In the image below,  $h_2$  and  $h_5$  are removed. Consequently, the calculation of  $y$  no longer depends on  $h_2$  and  $h_5$  and their respective gradient also vanishes when performing backprop. In this way,

the calculation of the output layer cannot be overly dependent on any one element of  $h_1, \dots, h_5$ . Intuitively, deep learning researchers often explain the intuition thusly: we do not want the network's output to depend too precariously on the exact activation pathway through the network. The original authors of the dropout technique described their intuition as an effort to prevent the *co-adaptation* of feature detectors.

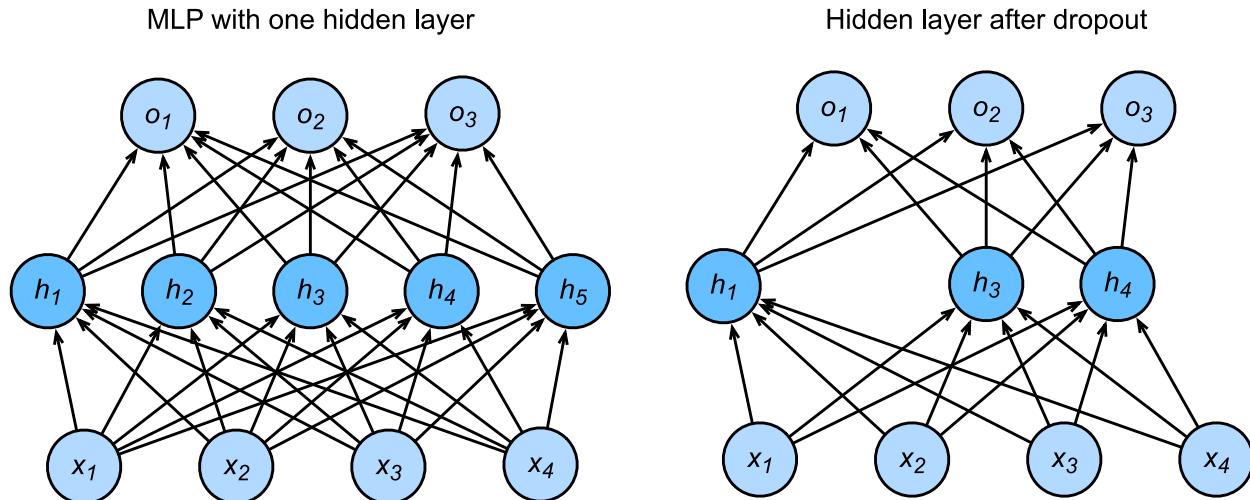


Fig. 6.6.1: MLP before and after dropout

At test time, we typically do not use dropout. However, we note that there are some exceptions: some researchers use dropout at test time as a heuristic approach for estimating the *confidence* of neural network predictions: if the predictions agree across many different dropout masks, then we might say that the network is more confident. For now we will put off the advanced topic of uncertainty estimation for subsequent chapters and volumes.

#### 6.6.4 Implementation from Scratch

To implement the dropout function for a single layer, we must draw as many samples from a Bernoulli (binary) random variable as our layer has dimensions, where the random variable takes value 1 (keep) with probability  $1 - p$  and 0 (drop) with probability  $p$ . One easy way to implement this is to first draw samples from the uniform distribution  $U[0, 1]$ . Then we can keep those nodes for which the corresponding sample is greater than  $p$ , dropping the rest.

In the following code, we implement a `dropout` function that drops out the elements in the NDArray input `X` with probability `drop_prob`, rescaling the remainder as described above (dividing the survivors by  $1 - \text{drop\_prob}$ ).

```
import d2l
from mxnet import autograd, gluon, init, nd
from mxnet.gluon import nn

def dropout(X, drop_prob):
    assert 0 <= drop_prob <= 1
    # In this case, all elements are dropped out
    if drop_prob == 1:
        return X.zeros_like()
    mask = nd.random.uniform(0, 1, X.shape) > drop_prob
    return mask * X / (1.0-drop_prob)
```

We can test out the `dropout` function on a few examples. In the following lines of code, we pass our input `X` through the dropout operation, with probabilities 0, 0.5, and 1, respectively.

```
X = nd.arange(16).reshape((2, 8))
print(dropout(X, 0))
print(dropout(X, 0.5))
print(dropout(X, 1))
```

```
[[ 0.  1.  2.  3.  4.  5.  6.  7.]
 [ 8.  9.  10. 11. 12. 13. 14. 15.]]
<NDArray 2x8 @cpu(0)>

[[ 0.  0.  0.  0.  8. 10. 12.  0.]
 [16.  0. 20. 22.  0.  0.  0. 30.]]
<NDArray 2x8 @cpu(0)>

[[0. 0. 0. 0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0. 0. 0. 0.]]
<NDArray 2x8 @cpu(0)>
```

## Defining Model Parameters

Again, we can use the Fashion-MNIST dataset, introduced in [Section 5.6](#). We will define a multilayer perceptron with two hidden layers. The two hidden layers both have 256 outputs.

```
num_inputs, num_outputs, num_hiddens1, num_hiddens2 = 784, 10, 256, 256

W1 = nd.random.normal(scale=0.01, shape=(num_inputs, num_hiddens1))
b1 = nd.zeros(num_hiddens1)
W2 = nd.random.normal(scale=0.01, shape=(num_hiddens1, num_hiddens2))
b2 = nd.zeros(num_hiddens2)
W3 = nd.random.normal(scale=0.01, shape=(num_hiddens2, num_outputs))
b3 = nd.zeros(num_outputs)

params = [W1, b1, W2, b2, W3, b3]
for param in params:
    param.attach_grad()
```

## Define the Model

The model defined below concatenates the fully-connected layer and the activation function ReLU, using dropout for the output of each activation function. We can set the dropout probability of each layer separately. It is generally recommended to set a lower dropout probability closer to the input layer. Below we set it to 0.2 and 0.5 for the first and second hidden layer respectively. By using the `is_training` function described in [Section 4.3](#), we can ensure that dropout is only active during training.

```
drop_prob1, drop_prob2 = 0.2, 0.5

def net(X):
    X = X.reshape((-1, num_inputs))
    H1 = (nd.dot(X, W1) + b1).relu()
    H2 = (nd.dot(H1, W2) + b2).relu()
    H3 = (nd.dot(H2, W3) + b3).relu()
    return H3
```

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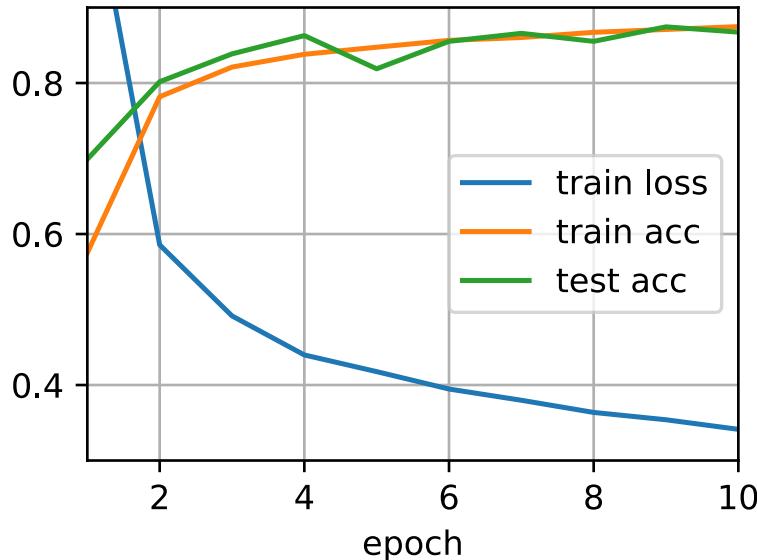
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```
# Use dropout only when training the model
if autograd.is_training():
    # Add a dropout layer after the first fully connected layer
    H1 = dropout(H1, drop_prob1)
H2 = (nd.dot(H1, W2) + b2).relu()
if autograd.is_training():
    # Add a dropout layer after the second fully connected layer
    H2 = dropout(H2, drop_prob2)
return nd.dot(H2, W3) + b3
```

## Training and Testing

This is similar to the training and testing of multilayer perceptrons described previously.

```
num_epochs, lr, batch_size = 10, 0.5, 256
loss = gluon.loss.SoftmaxCrossEntropyLoss()
train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size)
d2l.train_ch3(net, train_iter, test_iter, loss, num_epochs,
    lambda batch_size: d2l.sgd(params, lr, batch_size))
```



### 6.6.5 Concise Implementation

Using Gluon, all we need to do is add a `Dropout` layer (also in the `nn` package) after each fully-connected layer, passing in the dropout probability as the only argument to its constructor. During training, the `Dropout` layer will randomly drop out outputs of the previous layer (or equivalently, the inputs to the subsequent layer) according to the specified dropout probability. When MXNet is not in training mode, the `Dropout` layer simply passes the data through during testing.

```
net = nn.Sequential()
net.add(nn.Dense(256, activation="relu"),
```

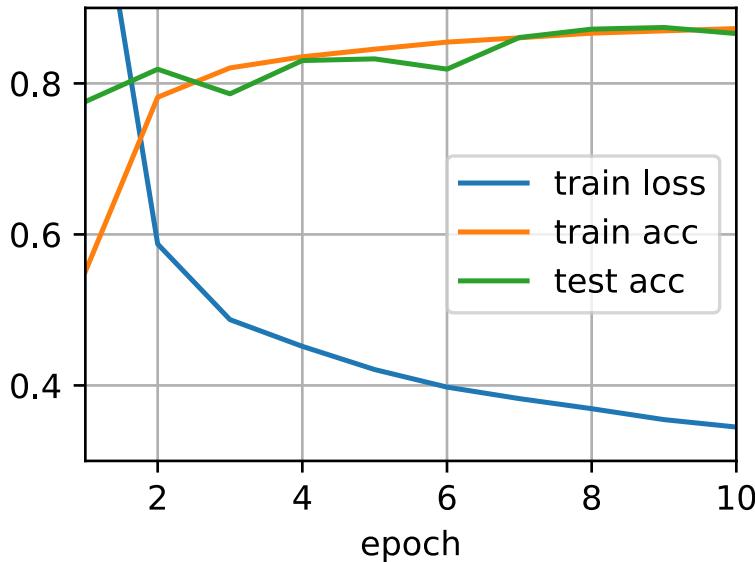
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```
# Add a dropout layer after the first fully connected layer
nn.Dropout(drop_prob1),
nn.Dense(256, activation="relu"),
# Add a dropout layer after the second fully connected layer
nn.Dropout(drop_prob2),
nn.Dense(10))
net.initialize(init.Normal(sigma=0.01))
```

Next, we train and test the model.

```
trainer = gluon.Trainer(net.collect_params(), 'sgd', {'learning_rate': lr})
d2l.train_ch3(net, train_iter, test_iter, loss, num_epochs, trainer)
```



## 6.6.6 Summary

- Beyond controlling the number of dimensions and the size of the weight vector, dropout is yet another tool to avoid overfitting. Often all three are used jointly.
- Dropout replaces an activation  $h$  with a random variable  $h'$  with expected value  $h$  and with variance given by the dropout probability  $p$ .
- Dropout is only used during training.

## 6.6.7 Exercises

1. Try out what happens if you change the dropout probabilities for layers 1 and 2. In particular, what happens if you switch the ones for both layers?
2. Increase the number of epochs and compare the results obtained when using dropout with those when not using it.
3. Compute the variance of the activation random variables after applying dropout.
4. Why should you typically not use dropout?

5. If changes are made to the model to make it more complex, such as adding hidden layer units, will the effect of using dropout to cope with overfitting be more obvious?
6. Using the model in this section as an example, compare the effects of using dropout and weight decay. What if dropout and weight decay are used at the same time?
7. What happens if we apply dropout to the individual weights of the weight matrix rather than the activations?
8. Replace the dropout activation with a random variable that takes on values of  $[0, \gamma/2, \gamma]$ . Can you design something that works better than the binary dropout function? Why might you want to use it? Why not?

### 6.6.8 Scan the QR Code to Discuss<sup>81</sup>



## 6.7 Forward Propagation, Backward Propagation, and Computational Graphs

In the previous sections, we used mini-batch stochastic gradient descent to train our models. When we implemented the algorithm, we only worried about the calculations involved in *forward propagation* through the model. In other words, we implemented the calculations required for the model to generate output corresponding to some given input, but when it came time to calculate the gradients of each of our parameters, we invoked the `backward` function, relying on the `autograd` module to figure out what to do.

The automatic calculation of gradients profoundly simplifies the implementation of deep learning algorithms. Before automatic differentiation, even small changes to complicated models would require recalculating lots of derivatives by hand. Even academic papers would too often have to allocate lots of page real estate to deriving update rules.

While we plan to continue relying on `autograd`, and we have already come a long way without even discussing how these gradients are calculated efficiently under the hood, it's important that you know how updates are actually calculated if you want to go beyond a shallow understanding of deep learning.

In this section, we'll peel back the curtain on some of the details of backward propagation (more commonly called *backpropagation* or *backprop*). To convey some insight for both the techniques and how they are implemented, we will rely on both mathematics and computational graphs to describe the mechanics behind neural network computations. To start, we will focus our exposition on a simple multilayer perceptron with a single hidden layer and  $\ell_2$  norm regularization.

### 6.7.1 Forward Propagation

Forward propagation refers to the calculation and storage of intermediate variables (including outputs) for the neural network within the models in the order from input layer to output layer. In the following, we

<sup>81</sup> <https://discuss.mxnet.io/t/2343>

work in detail through the example of a deep network with one hidden layer step by step. This is a bit tedious but it will serve us well when discussing what really goes on when we call `backward`.

For the sake of simplicity, let's assume that the input example is  $\mathbf{x} \in \mathbb{R}^d$  and there is no bias term. Here the intermediate variable is:

$$\mathbf{z} = \mathbf{W}^{(1)}\mathbf{x} \quad (6.7.1)$$

$\mathbf{W}^{(1)} \in \mathbb{R}^{h \times d}$  is the weight parameter of the hidden layer. After entering the intermediate variable  $\mathbf{z} \in \mathbb{R}^h$  into the activation function  $\phi$  operated by the basic elements, we will obtain a hidden layer variable with the vector length of  $h$ ,

$$\mathbf{h} = \phi(\mathbf{z}). \quad (6.7.2)$$

The hidden variable  $\mathbf{h}$  is also an intermediate variable. Assuming the parameters of the output layer only possess a weight of  $\mathbf{W}^{(2)} \in \mathbb{R}^{q \times h}$ , we can obtain an output layer variable with a vector length of  $q$ :

$$\mathbf{o} = \mathbf{W}^{(2)}\mathbf{h}. \quad (6.7.3)$$

Assuming the loss function is  $l$  and the example label is  $y$ , we can then calculate the loss term for a single data example,

$$L = l(\mathbf{o}, y). \quad (6.7.4)$$

According to the definition of  $\ell_2$  norm regularization, given the hyper-parameter  $\lambda$ , the regularization term is

$$s = \frac{\lambda}{2} \left( \|\mathbf{W}^{(1)}\|_F^2 + \|\mathbf{W}^{(2)}\|_F^2 \right), \quad (6.7.5)$$

where the Frobenius norm of the matrix is equivalent to the calculation of the  $L_2$  norm after flattening the matrix to a vector. Finally, the model's regularized loss on a given data example is

$$J = L + s. \quad (6.7.6)$$

We refer to  $J$  as the objective function of a given data example and refer to it as the ‘objective function’ in the following discussion.

## 6.7.2 Computational Graph of Forward Propagation

Plotting computational graphs helps us visualize the dependencies of operators and variables within the calculation. The figure below contains the graph associated with the simple network described above. The lower-left corner signifies the input and the upper right corner the output. Notice that the direction of the arrows (which illustrate data flow) are primarily rightward and upward.

## 6.7.3 Backpropagation

Backpropagation refers to the method of calculating the gradient of neural network parameters. In general, back propagation calculates and stores the intermediate variables of an objective function related to each layer of the neural network and the gradient of the parameters in the order of the output layer to the input layer according to the ‘chain rule’ in calculus. Assume that we have functions  $Y = f(X)$  and  $Z = g(Y) = g \circ f(X)$ , in which the input and the output  $X, Y, Z$  are tensors of arbitrary shapes. By using the chain rule, we can compute the derivative of  $Z$  wrt.  $X$  via

$$\frac{\partial Z}{\partial X} = \text{prod} \left( \frac{\partial Z}{\partial Y}, \frac{\partial Y}{\partial X} \right). \quad (6.7.7)$$

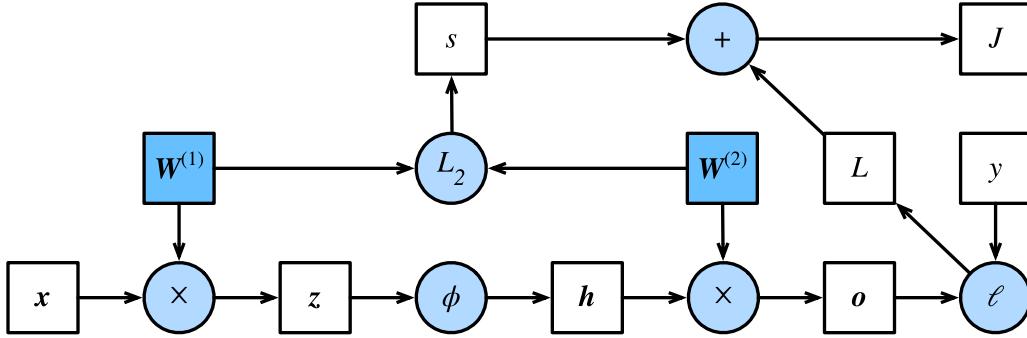


Fig. 6.7.1: Computational Graph

Here we use the prod operator to multiply its arguments after the necessary operations, such as transposition and swapping input positions have been carried out. For vectors, this is straightforward: it is simply matrix-matrix multiplication and for higher dimensional tensors we use the appropriate counterpart. The operator prod hides all the notation overhead.

The parameters of the simple network with one hidden layer are  $\mathbf{W}^{(1)}$  and  $\mathbf{W}^{(2)}$ . The objective of back-propagation is to calculate the gradients  $\partial J / \partial \mathbf{W}^{(1)}$  and  $\partial J / \partial \mathbf{W}^{(2)}$ . To accomplish this, we will apply the chain rule and calculate, in turn, the gradient of each intermediate variable and parameter. The order of calculations are reversed relative to those performed in forward propagation, since we need to start with the outcome of the compute graph and work our way towards the parameters. The first step is to calculate the gradients of the objective function  $J = L + s$  with respect to the loss term  $L$  and the regularization term  $s$ .

$$\frac{\partial J}{\partial L} = 1 \text{ and } \frac{\partial J}{\partial s} = 1 \quad (6.7.8)$$

Next, we compute the gradient of the objective function with respect to variable of the output layer  $\mathbf{o}$  according to the chain rule.

$$\frac{\partial J}{\partial \mathbf{o}} = \text{prod} \left( \frac{\partial J}{\partial L}, \frac{\partial L}{\partial \mathbf{o}} \right) = \frac{\partial L}{\partial \mathbf{o}} \in \mathbb{R}^q \quad (6.7.9)$$

Next, we calculate the gradients of the regularization term with respect to both parameters.

$$\frac{\partial s}{\partial \mathbf{W}^{(1)}} = \lambda \mathbf{W}^{(1)} \text{ and } \frac{\partial s}{\partial \mathbf{W}^{(2)}} = \lambda \mathbf{W}^{(2)} \quad (6.7.10)$$

Now we are able calculate the gradient  $\partial J / \partial \mathbf{W}^{(2)} \in \mathbb{R}^{q \times h}$  of the model parameters closest to the output layer. Using the chain rule yields:

$$\frac{\partial J}{\partial \mathbf{W}^{(2)}} = \text{prod} \left( \frac{\partial J}{\partial \mathbf{o}}, \frac{\partial \mathbf{o}}{\partial \mathbf{W}^{(2)}} \right) + \text{prod} \left( \frac{\partial J}{\partial s}, \frac{\partial s}{\partial \mathbf{W}^{(2)}} \right) = \frac{\partial J}{\partial \mathbf{o}} \mathbf{h}^\top + \lambda \mathbf{W}^{(2)} \quad (6.7.11)$$

To obtain the gradient with respect to  $\mathbf{W}^{(1)}$  we need to continue backpropagation along the output layer to the hidden layer. The gradient with respect to the hidden layer's outputs  $\partial J / \partial \mathbf{h} \in \mathbb{R}^h$  is given by

$$\frac{\partial J}{\partial \mathbf{h}} = \text{prod} \left( \frac{\partial J}{\partial \mathbf{o}}, \frac{\partial \mathbf{o}}{\partial \mathbf{h}} \right) = \mathbf{W}^{(2)\top} \frac{\partial J}{\partial \mathbf{o}}. \quad (6.7.12)$$

Since the activation function  $\phi$  applies element-wise, calculating the gradient  $\partial J / \partial \mathbf{z} \in \mathbb{R}^h$  of the intermediate variable  $\mathbf{z}$  requires that we use the element-wise multiplication operator, which we denote by  $\odot$ .

$$\frac{\partial J}{\partial \mathbf{z}} = \text{prod} \left( \frac{\partial J}{\partial \mathbf{h}}, \frac{\partial \mathbf{h}}{\partial \mathbf{z}} \right) = \frac{\partial J}{\partial \mathbf{h}} \odot \phi'(\mathbf{z}). \quad (6.7.13)$$

Finally, we can obtain the gradient  $\partial J / \partial \mathbf{W}^{(1)} \in \mathbb{R}^{h \times d}$  of the model parameters closest to the input layer. According to the chain rule, we get

$$\frac{\partial J}{\partial \mathbf{W}^{(1)}} = \text{prod} \left( \frac{\partial J}{\partial \mathbf{z}}, \frac{\partial \mathbf{z}}{\partial \mathbf{W}^{(1)}} \right) + \text{prod} \left( \frac{\partial J}{\partial s}, \frac{\partial s}{\partial \mathbf{W}^{(1)}} \right) = \frac{\partial J}{\partial \mathbf{z}} \mathbf{x}^\top + \lambda \mathbf{W}^{(1)}. \quad (6.7.14)$$

### 6.7.4 Training a Model

When training networks, forward and backward propagation depend on each other. In particular, for forward propagation, we traverse the compute graph in the direction of dependencies and compute all the variables on its path. These are then used for backpropagation where the compute order on the graph is reversed. One of the consequences is that we need to retain the intermediate values until backpropagation is complete. This is also one of the reasons why backpropagation requires significantly more memory than plain ‘inference’—we end up computing tensors as gradients and need to retain all the intermediate variables to invoke the chain rule. Another reason is that we typically train with minibatches containing more than one variable, thus more intermediate activations need to be stored.

### 6.7.5 Summary

- Forward propagation sequentially calculates and stores intermediate variables within the compute graph defined by the neural network. It proceeds from input to output layer.
- Back propagation sequentially calculates and stores the gradients of intermediate variables and parameters within the neural network in the reversed order.
- When training deep learning models, forward propagation and back propagation are interdependent.
- Training requires significantly more memory and storage.

### 6.7.6 Exercises

1. Assume that the inputs  $\mathbf{x}$  are matrices. What is the dimensionality of the gradients?
2. Add a bias to the hidden layer of the model described in this chapter.
  - Draw the corresponding compute graph.
  - Derive the forward and backward propagation equations.
3. Compute the memory footprint for training and inference in model described in the current chapter.
4. Assume that you want to compute *second* derivatives. What happens to the compute graph? Is this a good idea?
5. Assume that the compute graph is too large for your GPU.
  - Can you partition it over more than one GPU?
  - What are the advantages and disadvantages over training on a smaller minibatch?

### 6.7.7 Scan the QR Code to Discuss<sup>82</sup>

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<sup>82</sup> <https://discuss.mxnet.io/t/2344>



## 6.8 Numerical Stability and Initialization

In the past few sections, each model that we implemented required initializing our parameters according to some specified distribution. However, until now, we glossed over the details, taking the initialization hyperparameters for granted. You might even have gotten the impression that these choices are not especially important. However, the choice of initialization scheme plays a significant role in neural network learning, and can prove essentially to maintaining numerical stability. Moreover, these choices can be tied up in interesting ways with the choice of the activation function. Which nonlinear activation function we choose, and how we decide to initialize our parameters can play a crucial role in making the optimization algorithm converge rapidly. Failure to be mindful of these issues can lead to either exploding or vanishing gradients. In this section, we delve into these topics with greater detail and discuss some useful heuristics that you may use frequently throughout your career in deep learning.

### 6.8.1 Vanishing and Exploding Gradients

Consider a deep network with  $d$  layers, input  $\mathbf{x}$  and output  $\mathbf{o}$ . Each layer satisfies:

$$\mathbf{h}^{t+1} = f_t(\mathbf{h}^t) \text{ and thus } \mathbf{o} = f_d \circ \dots \circ f_1(\mathbf{x}) \quad (6.8.1)$$

If all activations and inputs are vectors, we can write the gradient of  $\mathbf{o}$  with respect to any set of parameters  $\mathbf{W}_t$  associated with the function  $f_t$  at layer  $t$  simply as

$$\partial_{\mathbf{W}_t} \mathbf{o} = \underbrace{\partial_{\mathbf{h}^{d-1}} \mathbf{h}^d}_{:= \mathbf{M}_d} \cdot \dots \cdot \underbrace{\partial_{\mathbf{h}^t} \mathbf{h}^{t+1}}_{:= \mathbf{M}_t} \underbrace{\partial_{\mathbf{W}_t} \mathbf{h}^t}_{:= \mathbf{v}_t}. \quad (6.8.2)$$

In other words, it is the product of  $d - t$  matrices  $\mathbf{M}_d \cdot \dots \cdot \mathbf{M}_t$  and the gradient vector  $\mathbf{v}_t$ . What happens is similar to the situation when we experienced numerical underflow when multiplying too many probabilities. At the time, we were able to mitigate the problem by switching from into log-space, i.e. by shifting the problem from the mantissa to the exponent of the numerical representation. Unfortunately the problem outlined in the equation above is much more serious: initially the matrices  $M_t$  may well have a wide variety of eigenvalues. They might be small, they might be large, and in particular, their product might well be *very large* or *very small*. This is not (only) a problem of numerical representation but it means that the optimization algorithm is bound to fail. It receives gradients that are either excessively large or excessively small. As a result the steps taken are either (i) excessively large (the *exploding gradient problem*), in which case the parameters blow up in magnitude rendering the model useless, or (ii) excessively small, (the *vanishing gradient problem*), in which case the parameters hardly move at all, and thus the learning process makes no progress.

#### Vanishing Gradients

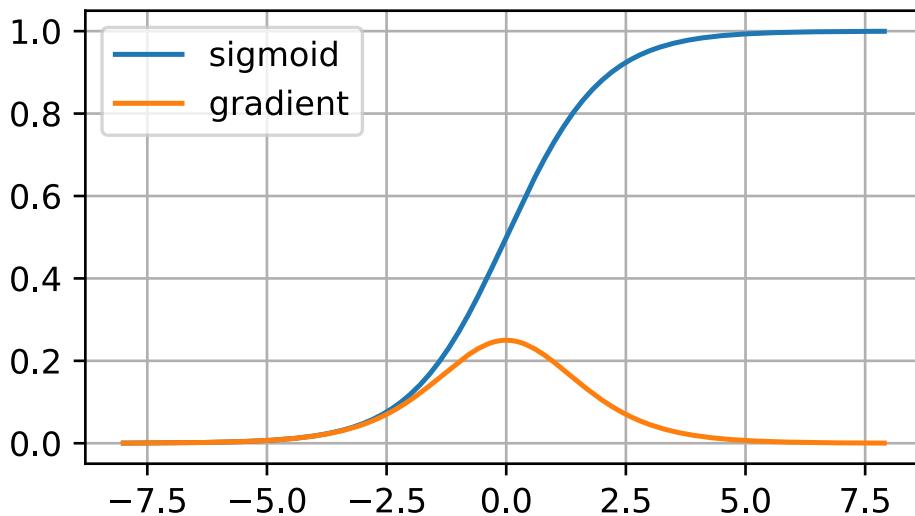
One major culprit in the vanishing gradient problem is the choices of the activation functions  $\sigma$  that are interleaved with the linear operations in each layer. Historically, the sigmoid function ( $1 + \exp(-x)$ ) (introduced in [Section 6.1](#)) was a popular choice owing to its similarity to a thresholding function. Since early artificial neural networks were inspired by biological neural networks, the idea of neurons that either fire

or do not fire (biological neurons do not partially fire) seemed appealing. Let's take a closer look at the function to see why picking it might be problematic vis-a-vis vanishing gradients.

```
%matplotlib inline
import d2l
from mxnet import nd, autograd

x = nd.arange(-8.0, 8.0, 0.1)
x.attach_grad()
with autograd.record():
    y = x.sigmoid()
y.backward()

d2l.plot(x, [y, x.grad], legend=['sigmoid', 'gradient'], figsize=(4.5, 2.5))
```



As we can see, the gradient of the sigmoid vanishes both when its inputs are large and when they are small. Moreover, when we execute backward propagation, due to the chain rule, this means that unless we are in the Goldilocks zone, where the inputs to most of the sigmoids are in the range of, say  $[-4, 4]$ , the gradients of the overall product may vanish. When we have many layers, unless we are especially careful, we are likely to find that our gradient is cut off at *some* layer. Before ReLUs ( $\max(0, x)$ ) were proposed as an alternative to squashing functions, this problem used to plague deep network training. As a consequence, ReLUs have become the default choice when designing activation functions in deep networks.

## Exploding Gradients

The opposite problem, when gradients explode, can be similarly vexing. To illustrate this a bit better, we draw 100 Gaussian random matrices and multiply them with some initial matrix. For the scale that we picked (the choice of the variance  $\sigma^2 = 1$ ), the matrix product explodes. If this were to happen to us with a deep network, we would have no realistic chance of getting a gradient descent optimizer to converge.

```
M = nd.random.normal(shape=(4,4))
print('A single matrix', M)
for i in range(100):
    M = nd.dot(M, nd.random.normal(shape=(4,4)))
```

(continues on next page)

(continued from previous page)

```

print('After multiplying 100 matrices', M)

A single matrix
[[ 2.2122064  0.7740038  1.0434405  1.1839255 ]
 [ 1.8917114 -1.2347414 -1.771029  -0.45138445]
 [ 0.57938355 -1.856082  -1.9768796 -0.20801921]
 [ 0.2444218  -0.03716067 -0.48774993 -0.02261727]]
<NDArray 4x4 @cpu(0)>
After multiplying 100 matrices
[[ 3.1575275e+20 -5.0052276e+19  2.0565092e+21 -2.3741922e+20]
 [-4.6332600e+20  7.3445046e+19 -3.0176513e+21  3.4838066e+20]
 [-5.8487235e+20  9.2711797e+19 -3.8092853e+21  4.3977330e+20]
 [-6.2947415e+19  9.9783660e+18 -4.0997977e+20  4.7331174e+19]]
<NDArray 4x4 @cpu(0)>

```

## Symmetry

Another problem in deep network design is the symmetry inherent in their parametrization. Assume that we have a deep network with one hidden layer with two units, say  $h_1$  and  $h_2$ . In this case, we could permute the weights  $\mathbf{W}_1$  of the first layer and likewise permute the weights of the output layer to obtain the same function. There is nothing special differentiating the first hidden unit vs the second hidden unit. In other words, we have permutation symmetry among the hidden units of each layer.

This is more than just a theoretical nuisance. Imagine what would happen if we initialized all of the parameters of some layer as  $\mathbf{W}_l = c$  for some constant  $c$ . In this case, the gradients for all dimensions are identical: thus not only would each unit take the same value, but it would receive the same update. Stochastic gradient descent would never break the symmetry on its own and we might never be able to realize the networks expressive power. The hidden layer would behave as if it had only a single unit. As an aside, note that while SGD would not break this symmetry, dropout regularization would!

### 6.8.2 Parameter Initialization

One way of addressing, or at least mitigating the issues raised above is through careful initialization of the weight vectors. This way we can ensure that (at least initially) the gradients do not vanish and that they maintain a reasonable scale where the network weights do not diverge. Additional care during optimization and suitable regularization ensures that things never get too bad.

#### Default Initialization

In the previous sections, e.g., in Section 5.3, we used `net.initialize(init.Normal(sigma=0.01))` to initialize the values of our weights. If the initialization method is not specified, such as `net.initialize()`, MXNet will use the default random initialization method: each element of the weight parameter is randomly sampled with a uniform distribution  $U[-0.07, 0.07]$  and the bias parameters are all set to 0. Both choices tend to work well in practice for moderate problem sizes.

## Xavier Initialization

Let's look at the scale distribution of the activations of the hidden units  $h_i$  for some layer. They are given by

$$h_i = \sum_{j=1}^{n_{\text{in}}} W_{ij} x_j \quad (6.8.3)$$

The weights  $W_{ij}$  are all drawn independently from the same distribution. Furthermore, let's assume that this distribution has zero mean and variance  $\sigma^2$  (this doesn't mean that the distribution has to be Gaussian, just that mean and variance need to exist). We don't really have much control over the inputs into the layer  $x_j$  but let's proceed with the somewhat unrealistic assumption that they also have zero mean and variance  $\gamma^2$  and that they're independent of  $\mathbf{W}$ . In this case, we can compute mean and variance of  $h_i$  as follows:

$$\begin{aligned} \mathbf{E}[h_i] &= \sum_{j=1}^{n_{\text{in}}} \mathbf{E}[W_{ij} x_j] = 0 \\ \mathbf{E}[h_i^2] &= \sum_{j=1}^{n_{\text{in}}} \mathbf{E}[W_{ij}^2 x_j^2] \\ &= \sum_{j=1}^{n_{\text{in}}} \mathbf{E}[W_{ij}^2] \mathbf{E}[x_j^2] \\ &= n_{\text{in}} \sigma^2 \gamma^2 \end{aligned} \quad (6.8.4)$$

One way to keep the variance fixed is to set  $n_{\text{in}}\sigma^2 = 1$ . Now consider backpropagation. There we face a similar problem, albeit with gradients being propagated from the top layers. That is, instead of  $\mathbf{W}\mathbf{w}$ , we need to deal with  $\mathbf{W}^\top \mathbf{g}$ , where  $\mathbf{g}$  is the incoming gradient from the layer above. Using the same reasoning as for forward propagation, we see that the gradients' variance can blow up unless  $n_{\text{out}}\sigma^2 = 1$ . This leaves us in a dilemma: we cannot possibly satisfy both conditions simultaneously. Instead, we simply try to satisfy:

$$\frac{1}{2}(n_{\text{in}} + n_{\text{out}})\sigma^2 = 1 \text{ or equivalently } \sigma = \sqrt{\frac{2}{n_{\text{in}} + n_{\text{out}}}}. \quad (6.8.5)$$

This is the reasoning underlying the eponymous Xavier initialization [18]. It works well enough in practice. For Gaussian random variables, the Xavier initialization picks a normal distribution with zero mean and variance  $\sigma^2 = 2/(n_{\text{in}} + n_{\text{out}})$ . For uniformly distributed random variables  $U[-a, a]$ , note that their variance is given by  $a^2/3$ . Plugging  $a^2/3$  into the condition on  $\sigma^2$  yields that we should initialize uniformly with  $U\left[-\sqrt{6/(n_{\text{in}} + n_{\text{out}})}, \sqrt{6/(n_{\text{in}} + n_{\text{out}})}\right]$ .

## Beyond

The reasoning above barely scratches the surface of modern approaches to parameter initialization. In fact, MXNet has an entire `mxnet.initializer` module implementing over a dozen different heuristics. Moreover, initialization continues to be a hot area of inquiry within research into the fundamental theory of neural network optimization. Some of these heuristics are especially suited for when parameters are tied (i.e., when parameters of in different parts the network are shared), for superresolution, sequence models, and related problems. We recommend that the interested reader take a closer look at what is offered as part of this module, and investigate the recent research on parameter initialization. Perhaps you may come across a recent clever idea and contribute its implementation to MXNet, or you may even invent your own scheme!

### 6.8.3 Summary

- Vanishing and exploding gradients are common issues in very deep networks, unless great care is taking to ensure that gradients and parameters remain well controlled.

- Initialization heuristics are needed to ensure that at least the initial gradients are neither too large nor too small.
- The ReLU addresses one of the vanishing gradient problems, namely that gradients vanish for very large inputs. This can accelerate convergence significantly.
- Random initialization is key to ensure that symmetry is broken before optimization.

#### 6.8.4 Exercises

1. Can you design other cases of symmetry breaking besides the permutation symmetry?
2. Can we initialize all weight parameters in linear regression or in softmax regression to the same value?
3. Look up analytic bounds on the eigenvalues of the product of two matrices. What does this tell you about ensuring that gradients are well conditioned?
4. If we know that some terms diverge, can we fix this after the fact? Look at the paper on LARS by You, Gitman and Ginsburg, 2017<sup>83</sup> for inspiration.

#### 6.8.5 Scan the QR Code to Discuss<sup>84</sup>



### 6.9 Considering the Environment

So far, we have worked through a number of hands-on implementations fitting machine learning models to a variety of datasets. And yet, until now we skated over the matter of where data comes from in the first place, and what we plan to ultimately *do* with the outputs from our models. Too often in the practice of machine learning, developers rush ahead with the development of models tossing these fundamental considerations aside.

Many failed machine learning deployments can be traced back to this situation. Sometimes the model does well as evaluated by test accuracy only to fail catastrophically in the real world when the distribution of data suddenly shifts. More insidiously, sometimes the very deployment of a model can be the catalyst which perturbs the data distribution. Say for example that we trained a model to predict loan defaults, finding that the choice of footwear was associated with risk of default (Oxfords indicate repayment, sneakers indicate default). We might be inclined to thereafter grant loans to all applicants wearing Oxfords and to deny all applicants wearing sneakers. But our ill-conceived leap from pattern recognition to decision-making and our failure to think critically about the environment might have disastrous consequences. For starters, as soon as we began making decisions based on footwear, customers would catch on and change their behavior. Before long, all applicants would be wearing Oxfords, and yet there would be no coinciding improvement in credit-worthiness. Think about this deeply because similar issues abound in the application of machine learning: by introducing our model-based decisions to the environment, we might break the model.

<sup>83</sup> <https://arxiv.org/pdf/1708.03888.pdf>

<sup>84</sup> <https://discuss.mxnet.io/t/2345>

In this chapter, we describe some common concerns and aim to get you started acquiring the critical thinking that you will need in order to detect these situations early, mitigate the damage, and use machine learning responsibly. Some of the solutions are simple (ask for the ‘right’ data) some are technically difficult (implement a reinforcement learning system), and others require that we enter the realm of philosophy and grapple with difficult questions concerning ethics and informed consent.

### 6.9.1 Distribution Shift

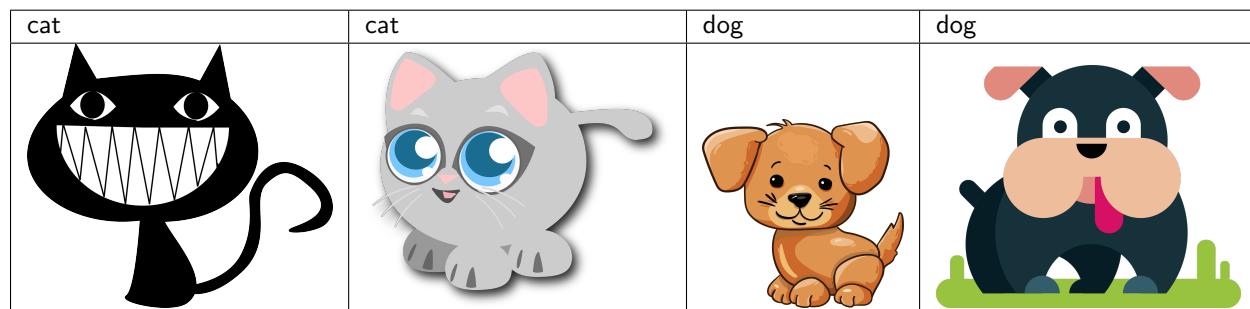
To begin, we return to the observational setting, putting aside for now the impacts of our actions on the environment. In the following sections, we take a deeper look at the various ways that data distributions might shift, and what might be done to salvage model performance. From the outset, we should warn that if the data-generating distribution  $p(\mathbf{x}, y)$  can shift in arbitrary ways at any point in time, then learning a robust classifier is impossible. In the most pathological case, if the label definitions themselves can change at a moment’s notice: if suddenly what we called “cats” are now dogs and what we previously called “dogs” are now in fact cats, without any perceptible change in the distribution of inputs  $p(\mathbf{x})$ , then there is nothing we could do to detect the change or to correct our classifier at test time. Fortunately, under some restricted assumptions on the ways our data might change in the future, principled algorithms can detect shift and possibly even adapt, achieving higher accuracy than if we naively continued to rely on our original classifier.

#### Covariate Shift

One of the best-studied forms of distribution shift is *covariate shift*. Here we assume that although the distribution of inputs may change over time, the labeling function, i.e., the conditional distribution  $p(y|\mathbf{x})$  does not change. While this problem is easy to understand its also easy to overlook it in practice. Consider the challenge of distinguishing cats and dogs. Our training data consists of images of the following kind:



At test time we are asked to classify the following images:



Obviously this is unlikely to work well. The training set consists of photos, while the test set contains only cartoons. The colors aren’t even realistic. Training on a dataset that looks substantially different from the

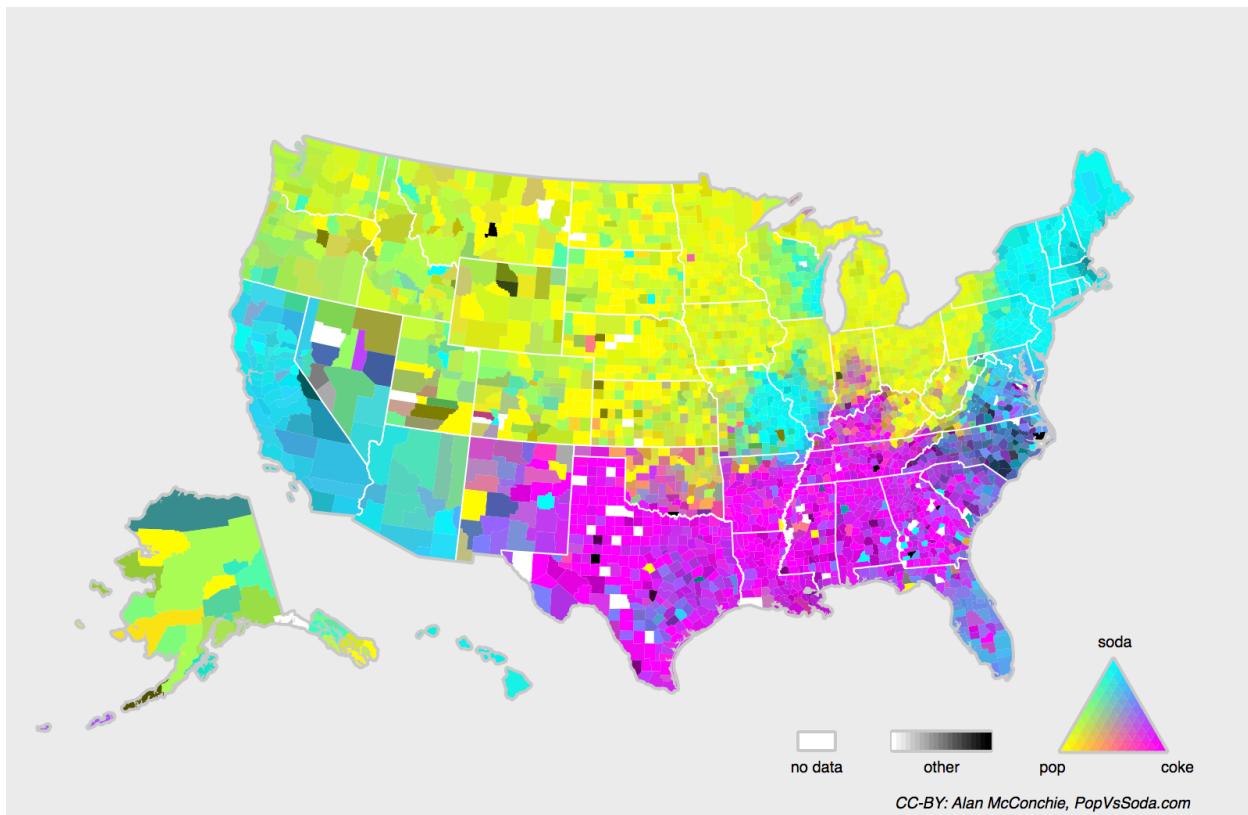
test set without some plan for how to adapt to the new domain is a bad idea. Unfortunately, this is a very common pitfall. Statisticians call this *covariate shift* because the root of the problem owed to a shift in the distribution of features (i.e., of *covariates*). Mathematically, we could say that  $p(\mathbf{x})$  changes but that  $p(y|\mathbf{x})$  remains unchanged. Although its usefulness is not restricted to this setting, when we believe  $\mathbf{x}$  causes  $y$ , covariate shift is usually the right assumption to be working with.

### Label Shift

The converse problem emerges when we believe that what drives the shift is a change in the marginal distribution over the labels  $p(y)$  but that the class-conditional distributions are invariant  $p(\mathbf{x}|y)$ . Label shift is a reasonable assumption to make when we believe that  $y$  causes  $\mathbf{x}$ . For example, commonly we want to predict a diagnosis given its manifestations. In this case we believe that the diagnosis causes the manifestations, i.e., diseases cause symptoms. Sometimes the label shift and covariate shift assumptions can hold simultaneously. For example, when the true labeling function is deterministic and unchanging, then covariate shift will always hold, including if label shift holds too. Interestingly, when we expect both label shift and covariate shift hold, it's often advantageous to work with the methods that flow from the label shift assumption. That's because these methods tend to involve manipulating objects that look like the label, which (in deep learning) tends to be comparatively easy compared to working with the objects that look like the input, which tends (in deep learning) to be a high-dimensional object.

### Concept Shift

One more related problem arises in *concept shift*, the situation in which the very label definitions change. This sounds weird—after all, a *cat* is a *cat*. Indeed the definition of a cat might not change, but can we say the same about soft drinks? It turns out that if we navigate around the United States, shifting the source of our data by geography, we'll find considerable concept shift regarding the definition of even this simple term:



If we were to build a machine translation system, the distribution  $p(y|x)$  might be different depending on our location. This problem can be tricky to spot. A saving grace is that often the  $p(y|x)$  only shifts gradually. Before we go into further detail and discuss remedies, we can discuss a number of situations where covariate and concept shift may not be so obvious.

## Examples

### Medical Diagnostics

Imagine that you want to design an algorithm to detect cancer. You collect data from healthy and sick people and you train your algorithm. It works fine, giving you high accuracy and you conclude that you're ready for a successful career in medical diagnostics. Not so fast...

Many things could go wrong. In particular, the distributions that you work with for training and those that you encounter in the wild might differ considerably. This happened to an unfortunate startup, that Alex had the opportunity to consult for many years ago. They were developing a blood test for a disease that affects mainly older men and they'd managed to obtain a fair amount of blood samples from patients. It is considerably more difficult, though, to obtain blood samples from healthy men (mainly for ethical reasons). To compensate for that, they asked a large number of students on campus to donate blood and they performed their test. Then they asked me whether I could help them build a classifier to detect the disease. I told them that it would be very easy to distinguish between both datasets with near-perfect accuracy. After all, the test subjects differed in age, hormone levels, physical activity, diet, alcohol consumption, and many more factors unrelated to the disease. This was unlikely to be the case with real patients: Their sampling procedure made it likely that an extreme case of covariate shift would arise between the *source* and *target* distributions, and at that, one that could not be corrected by conventional means. In other words, training and test data were so different that nothing useful could be done and they had wasted significant amounts of money.

### Self Driving Cars

Say a company wanted to build a machine learning system for self-driving cars. One of the key components is a roadside detector. Since real annotated data is expensive to get, they had the (smart and questionable) idea to use synthetic data from a game rendering engine as additional training data. This worked really well on ‘test data’ drawn from the rendering engine. Alas, inside a real car it was a disaster. As it turned out, the roadside had been rendered with a very simplistic texture. More importantly, *all* the roadside had been rendered with the *same* texture and the roadside detector learned about this ‘feature’ very quickly.

A similar thing happened to the US Army when they first tried to detect tanks in the forest. They took aerial photographs of the forest without tanks, then drove the tanks into the forest and took another set of pictures. The so-trained classifier worked ‘perfectly’. Unfortunately, all it had learned was to distinguish trees with shadows from trees without shadows—the first set of pictures was taken in the early morning, the second one at noon.

### Nonstationary distributions

A much more subtle situation arises when the distribution changes slowly and the model is not updated adequately. Here are some typical cases:

- We train a computational advertising model and then fail to update it frequently (e.g. we forget to incorporate that an obscure new device called an iPad was just launched).
- We build a spam filter. It works well at detecting all spam that we’ve seen so far. But then the spammers wisen up and craft new messages that look unlike anything we’ve seen before.

- We build a product recommendation system. It works throughout the winter... but then it keeps on recommending Santa hats long after Christmas.

## More Anecdotes

- We build a face detector. It works well on all benchmarks. Unfortunately it fails on test data - the offending examples are close-ups where the face fills the entire image (no such data was in the training set).
- We build a web search engine for the USA market and want to deploy it in the UK.
- We train an image classifier by compiling a large dataset where each among a large set of classes is equally represented in the dataset, say 1000 categories, represented by 1000 images each. Then we deploy the system in the real world, where the actual label distribution of photographs is decidedly non-uniform.

In short, there are many cases where training and test distributions  $p(\mathbf{x}, y)$  are different. In some cases, we get lucky and the models work despite covariate, label, or concept shift. In other cases, we can do better by employing principled strategies to cope with the shift. The remainder of this section grows considerably more technical. The impatient reader could continue on to the next section as this material is not prerequisite to subsequent concepts.

## Covariate Shift Correction

Assume that we want to estimate some dependency  $p(y|\mathbf{x})$  for which we have labeled data  $(\mathbf{x}_i, y_i)$ . Unfortunately, the observations  $x_i$  are drawn from some *target* distribution  $q(\mathbf{x})$  rather than the *source* distribution  $p(\mathbf{x})$ . To make progress, we need to reflect about what exactly is happening during training: we iterate over training data and associated labels  $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$  and update the weight vectors of the model after every minibatch. We sometimes additionally apply some penalty to the parameters, using weight decay, dropout, or some other related technique. This means that we largely minimize the loss on the training.

$$\underset{w}{\text{minimize}} \frac{1}{n} \sum_{i=1}^n l(x_i, y_i, f(x_i)) + \text{some penalty}(w) \quad (6.9.1)$$

Statisticians call the first term an *empirical average*, i.e., an average computed over the data drawn from  $p(x)p(y|x)$ . If the data is drawn from the ‘wrong’ distribution  $q$ , we can correct for that by using the following simple identity:

$$\begin{aligned} \int p(\mathbf{x})f(\mathbf{x})dx &= \int p(\mathbf{x})f(\mathbf{x})\frac{q(\mathbf{x})}{q(\mathbf{x})}dx \\ &= \int q(\mathbf{x})f(\mathbf{x})\frac{p(\mathbf{x})}{q(\mathbf{x})}dx \end{aligned} \quad (6.9.2)$$

In other words, we need to re-weight each instance by the ratio of probabilities that it would have been drawn from the correct distribution  $\beta(\mathbf{x}) := p(\mathbf{x})/q(\mathbf{x})$ . Alas, we do not know that ratio, so before we can do anything useful we need to estimate it. Many methods are available, including some fancy operator-theoretic approaches that attempt to recalibrate the expectation operator directly using a minimum-norm or a maximum entropy principle. Note that for any such approach, we need samples drawn from both distributions—the ‘true’  $p$ , e.g., by access to training data, and the one used for generating the training set  $q$  (the latter is trivially available). Note however, that we only need samples  $\mathbf{x} \sim q(\mathbf{x})$ ; we do not need to access labels  $y \sim q(y)$ .

In this case, there exists a very effective approach that will give almost as good results: logistic regression. This is all that is needed to compute estimate probability ratios. We learn a classifier to distinguish between data drawn from  $p(\mathbf{x})$  and data drawn from  $q(x)$ . If it is impossible to distinguish between the two

distributions then it means that the associated instances are equally likely to come from either one of the two distributions. On the other hand, any instances that can be well discriminated should be significantly over/underweighted accordingly. For simplicity's sake assume that we have an equal number of instances from both distributions, denoted by  $\mathbf{x}_i \sim p(\mathbf{x})$  and  $\mathbf{x}'_i \sim q(\mathbf{x})$  respectively. Now denote by  $z_i$  labels which are 1 for data drawn from  $p$  and -1 for data drawn from  $q$ . Then the probability in a mixed dataset is given by

$$p(z = 1|\mathbf{x}) = \frac{p(\mathbf{x})}{p(\mathbf{x}) + q(\mathbf{x})} \text{ and hence } \frac{p(z = 1|\mathbf{x})}{p(z = -1|\mathbf{x})} = \frac{p(\mathbf{x})}{q(\mathbf{x})} \quad (6.9.3)$$

Hence, if we use a logistic regression approach where  $p(z = 1|\mathbf{x}) = \frac{1}{1 + \exp(-f(\mathbf{x}))}$  it follows that

$$\beta(\mathbf{x}) = \frac{1/(1 + \exp(-f(\mathbf{x})))}{\exp(-f(\mathbf{x})/(1 + \exp(-f(\mathbf{x}))))} = \exp(f(\mathbf{x})) \quad (6.9.4)$$

As a result, we need to solve two problems: first one to distinguish between data drawn from both distributions, and then a reweighted minimization problem where we weigh terms by  $\beta$ , e.g. via the head gradients. Here's a prototypical algorithm for that purpose which uses an unlabeled training set  $X$  and test set  $Z$ :

1. Generate training set with  $\{(\mathbf{x}_i, -1) \dots (\mathbf{z}_j, 1)\}$
2. Train binary classifier using logistic regression to get function  $f$
3. Weigh training data using  $\beta_i = \exp(f(\mathbf{x}_i))$  or better  $\beta_i = \min(\exp(f(\mathbf{x}_i)), c)$
4. Use weights  $\beta_i$  for training on  $X$  with labels  $Y$

Note that this method relies on a crucial assumption. For this scheme to work, we need that each data point in the target (test time) distribution had nonzero probability of occurring at training time. If we find a point where  $q(\mathbf{x}) > 0$  but  $p(\mathbf{x}) = 0$ , then the corresponding importance weight should be infinity.

**Generative Adversarial Networks** use a very similar idea to that described above to engineer a *data generator* that outputs data that cannot be distinguished from examples sampled from a reference dataset. In these approaches, we use one network,  $f$  to distinguish real versus fake data and a second network  $g$  that tries to fool the discriminator  $f$  into accepting fake data as real. We will discuss this in much more detail later.

## Label Shift Correction

For the discussion of label shift, we'll assume for now that we are dealing with a  $k$ -way multiclass classification task. When the distribution of labels shifts over time  $p(y) \neq q(y)$  but the class-conditional distributions stay the same  $p(\mathbf{x}) = q(\mathbf{x})$ , our importance weights will correspond to the label likelihood ratios  $q(y)/p(y)$ . One nice thing about label shift is that if we have a reasonably good model (on the source distribution) then we can get consistent estimates of these weights without ever having to deal with the ambient dimension (in deep learning, the inputs are often high-dimensional perceptual objects like images, while the labels are often easier to work, say vectors whose length corresponds to the number of classes).

To estimate calculate the target label distribution, we first take our reasonably good off the shelf classifier (typically trained on the training data) and compute its confusion matrix using the validation set (also from the training distribution). The confusion matrix  $C$ , is simply a  $k \times k$  matrix where each column corresponds to the *actual* label and each row corresponds to our model's predicted label. Each cell's value  $c_{ij}$  is the fraction of predictions where the true label was  $j$  and our model predicted  $y$ .

Now we can't calculate the confusion matrix on the target data directly, because we don't get to see the labels for the examples that we see in the wild, unless we invest in a complex real-time annotation pipeline. What we can do, however, is average all of our models predictions at test time together, yielding the mean model output  $\mu_y$ .

It turns out that under some mild conditions—if our classifier was reasonably accurate in the first place, if the target data contains only classes of images that we've seen before, and if the label shift assumption holds in the first place (far the strongest assumption here), then we can recover the test set label distribution by solving a simple linear system  $C \cdot q(y) = \mu_y$ . If our classifier is sufficiently accurate to begin with, then the confusion  $C$  will be invertible, and we get a solution  $q(y) = C^{-1}\mu_y$ . Here we abuse notation a bit, using  $q(y)$  to denote the vector of label frequencies. Because we observe the labels on the source data, it's easy to estimate the distribution  $p(y)$ . Then for any training example  $i$  with label  $y$ , we can take the ratio of our estimates  $\hat{q}(y)/\hat{p}(y)$  to calculate the weight  $w_i$ , and plug this into the weighted risk minimization algorithm above.

### Concept Shift Correction

Concept shift is much harder to fix in a principled manner. For instance, in a situation where suddenly the problem changes from distinguishing cats from dogs to one of distinguishing white from black animals, it will be unreasonable to assume that we can do much better than just collecting new labels and training from scratch. Fortunately, in practice, such extreme shifts are rare. Instead, what usually happens is that the task keeps on changing slowly. To make things more concrete, here are some examples:

- In computational advertising, new products are launched, old products become less popular. This means that the distribution over ads and their popularity changes gradually and any click-through rate predictor needs to change gradually with it.
- Traffic cameras lenses degrade gradually due to environmental wear, affecting image quality progressively.
- News content changes gradually (i.e. most of the news remains unchanged but new stories appear).

In such cases, we can use the same approach that we used for training networks to make them adapt to the change in the data. In other words, we use the existing network weights and simply perform a few update steps with the new data rather than training from scratch.

### 6.9.2 A Taxonomy of Learning Problems

Armed with knowledge about how to deal with changes in  $p(x)$  and in  $p(y|x)$ , we can now consider some other aspects of machine learning problems formulation.

- **Batch Learning.** Here we have access to training data and labels  $\{(x_1, y_1), \dots, (x_n, y_n)\}$ , which we use to train a network  $f(x, w)$ . Later on, we deploy this network to score new data  $(x, y)$  drawn from the same distribution. This is the default assumption for any of the problems that we discuss here. For instance, we might train a cat detector based on lots of pictures of cats and dogs. Once we trained it, we ship it as part of a smart catdoor computer vision system that lets only cats in. This is then installed in a customer's home and is never updated again (barring extreme circumstances).
- **Online Learning.** Now imagine that the data  $(x_i, y_i)$  arrives one sample at a time. More specifically, assume that we first observe  $x_i$ , then we need to come up with an estimate  $f(x_i, w)$  and only once we've done this, we observe  $y_i$  and with it, we receive a reward (or incur a loss), given our decision. Many real problems fall into this category. E.g. we need to predict tomorrow's stock price, this allows us to trade based on that estimate and at the end of the day we find out whether our estimate allowed us to make a profit. In other words, we have the following cycle where we are continuously improving our model given new observations.

$$\text{model } f_t \rightarrow \text{data } x_t \rightarrow \text{estimate } f_t(x_t) \rightarrow \text{observation } y_t \rightarrow \text{loss } l(y_t, f_t(x_t)) \rightarrow \text{model } f_{t+1} \quad (6.9.5)$$

- **Bandits.** They are a *special case* of the problem above. While in most learning problems we have a continuously parametrized function  $f$  where we want to learn its parameters (e.g. a deep network), in a bandit problem we only have a finite number of arms that we can pull (i.e. a finite number of

actions that we can take). It is not very surprising that for this simpler problem stronger theoretical guarantees in terms of optimality can be obtained. We list it mainly since this problem is often (confusingly) treated as if it were a distinct learning setting.

- **Control (and nonadversarial Reinforcement Learning).** In many cases the environment remembers what we did. Not necessarily in an adversarial manner but it'll just remember and the response will depend on what happened before. E.g. a coffee boiler controller will observe different temperatures depending on whether it was heating the boiler previously. PID (proportional integral derivative) controller algorithms are a popular choice there. Likewise, a user's behavior on a news site will depend on what we showed him previously (e.g. he will read most news only once). Many such algorithms form a model of the environment in which they act such as to make their decisions appear less random (i.e. to reduce variance).
- **Reinforcement Learning.** In the more general case of an environment with memory, we may encounter situations where the environment is trying to *cooperate* with us (cooperative games, in particular for non-zero-sum games), or others where the environment will try to *win*. Chess, Go, Backgammon or StarCraft are some of the cases. Likewise, we might want to build a good controller for autonomous cars. The other cars are likely to respond to the autonomous car's driving style in nontrivial ways, e.g. trying to avoid it, trying to cause an accident, trying to cooperate with it, etc.

One key distinction between the different situations above is that the same strategy that might have worked throughout in the case of a stationary environment, might not work throughout when the environment can adapt. For instance, an arbitrage opportunity discovered by a trader is likely to disappear once he starts exploiting it. The speed and manner at which the environment changes determines to a large extent the type of algorithms that we can bring to bear. For instance, if we *know* that things may only change slowly, we can force any estimate to change only slowly, too. If we know that the environment might change instantaneously, but only very infrequently, we can make allowances for that. These types of knowledge are crucial for the aspiring data scientist to deal with concept shift, i.e. when the problem that he is trying to solve changes over time.

### 6.9.3 Fairness, Accountability, and Transparency in machine Learning

Finally, it's important to remember that when you deploy machine learning systems you aren't simply minimizing negative log likelihood or maximizing accuracy—you are automating some kind of decision process. Often the automated decision-making systems that we deploy can have consequences for those subject to its decisions. If we are deploying a medical diagnostic system, we need to know for which populations it may work and which it may not. Overlooking foreseeable risks to the welfare of a subpopulation would run afoul of basic ethical principles. Moreover, “accuracy” is seldom the right metric. When translating predictions into actions we'll often want to take into account the potential cost sensitivity of erring in various ways. If one way that you might classify an image could be perceived as a racial slight, while misclassification to a different category would be harmless, then you might want to adjust your thresholds accordingly, accounting for societal values in designing the decision-making protocol. We also want to be careful about how prediction systems can lead to feedback loops. For example, if prediction systems are applied naively to predictive policing, allocating patrol officers accordingly, a vicious cycle might emerge. Neighborhoods that have more crimes, get more patrols, get more crimes discovered, get more training data, get yet more confident predictions, leading to even more patrols, even more crimes discovered, etc. Additionally, we want to be careful about whether we are addressing the right problem in the first place. Predictive algorithms now play an outsize role in mediating the dissemination of information. Should what news someone is exposed to be determined by which Facebook pages they have *Liked*? These are just a few among the many profound ethical dilemmas that you might encounter in a career in machine learning.

### 6.9.4 Summary

- In many cases training and test set do not come from the same distribution. This is called covariate shift.
- Covariate shift can be detected and corrected if the shift isn't too severe. Failure to do so leads to nasty surprises at test time.
- In some cases the environment *remembers* what we did and will respond in unexpected ways. We need to account for that when building models.

### 6.9.5 Exercises

1. What could happen when we change the behavior of a search engine? What might the users do? What about the advertisers?
2. Implement a covariate shift detector. Hint - build a classifier.
3. Implement a covariate shift corrector.
4. What could go wrong if training and test set are very different? What would happen to the sample weights?

### 6.9.6 Scan the QR Code to Discuss<sup>85</sup>



## 6.10 Predicting House Prices on Kaggle

In the previous sections, we introduced the basic tools for building deep networks and performing capacity control via dimensionality-reduction, weight decay and dropout. You are now ready to put all this knowledge into practice by participating in a Kaggle competition. [Predicting house prices](#)<sup>86</sup> is a great place to start: the data is reasonably generic and doesn't have the kind of rigid structure that might require specialized models the way images or audio might. This dataset, collected by [Bart de Cock](#)<sup>87</sup> in 2011, is considerably larger than the famous the [Boston housing dataset](#)<sup>88</sup> of Harrison and Rubinfeld (1978). It boasts both more examples and more features, covering house prices in Ames, IA from the period of 2006-2010.

In this section, we will walk you through details of data preprocessing, model design, hyperparameter selection and tuning. We hope that through a hands-on approach, you will be able to observe the effects of capacity control, feature extraction, etc. in practice. This experience is vital to gaining intuition as a data scientist.

<sup>85</sup> <https://discuss.mxnet.io/t/2347>

<sup>86</sup> <https://www.kaggle.com/c/house-prices-advanced-regression-techniques>

<sup>87</sup> <http://jse.amstat.org/v19n3/decock.pdf>

<sup>88</sup> <https://archive.ics.uci.edu/ml/machine-learning-databases/housing/housing.names>

### 6.10.1 Kaggle

Kaggle<sup>89</sup> is a popular platform for machine learning competitions. It combines data, code and users in a way to allow for both collaboration and competition. While leaderboard chasing can sometimes get out of control, there's also a lot to be said for the objectivity in a platform that provides fair and direct quantitative comparisons between your approaches and those devised by your competitors. Moreover, you can checkout the code from (some) other competitors' submissions and pick apart their methods to learn new techniques. If you want to participate in one of the competitions, you need to register for an account (do this now!).

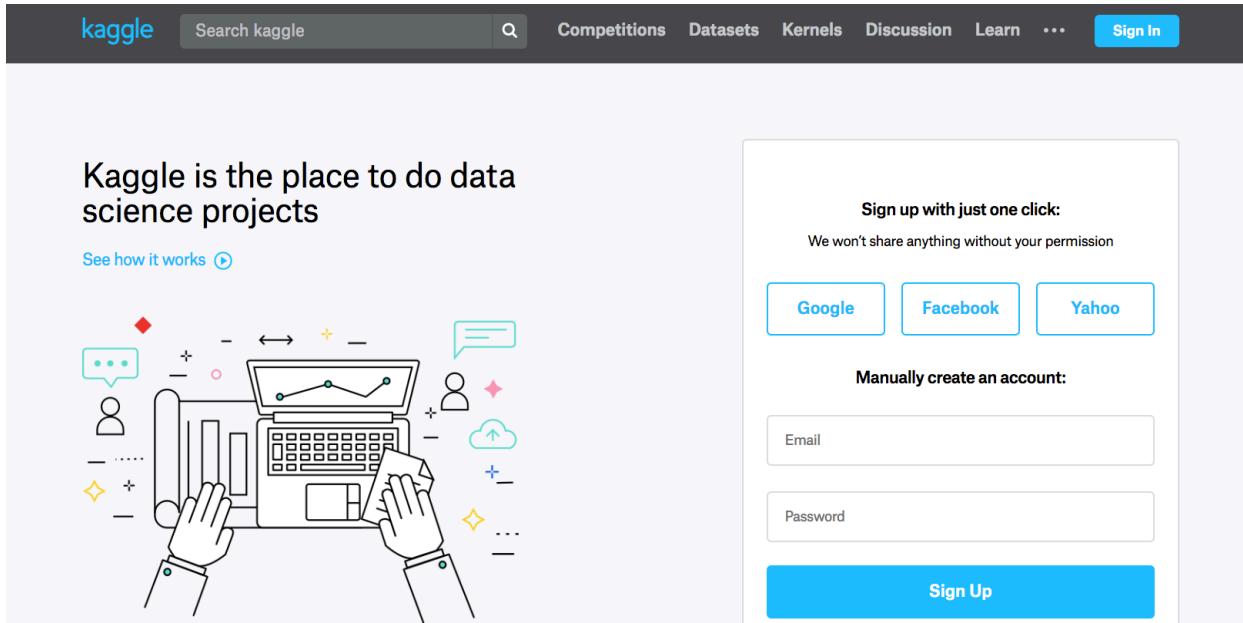


Fig. 6.10.1: Kaggle website

On the House Prices Prediction page, you can find the data set (under the data tab), submit predictions, see your ranking, etc., The URL is right here:

<https://www.kaggle.com/c/house-prices-advanced-regression-techniques>

### 6.10.2 Accessing and Reading Data Sets

Note that the competition data is separated into training and test sets. Each record includes the property value of the house and attributes such as street type, year of construction, roof type, basement condition, etc. The features represent multiple datatypes. Year of construction, for example, is represented with integers roof type is a discrete categorical feature, other features are represented with floating point numbers. And here is where reality comes in: for some examples, some data is altogether missing with the missing value marked simply as 'na'. The price of each house is included for the training set only (it's a competition after all). You can partition the training set to create a validation set, but you'll only find out how you perform on the official test set when you upload your predictions and receive your score. The 'Data' tab on the competition tab has links to download the data.

We will read and process the data using `pandas`, an efficient data analysis toolkit<sup>90</sup>, so you will want to make sure that you have `pandas` installed before proceeding further. Fortunately, if you're reading in Jupyter, we can install `pandas` without even leaving the notebook.

<sup>89</sup> <https://www.kaggle.com>

<sup>90</sup> <http://pandas.pydata.org/pandas-docs/stable/>

The screenshot shows the Kaggle competition page for 'House Prices: Advanced Regression Techniques'. At the top left is a red house icon with a yellow 'SOLD' sign. The title 'House Prices: Advanced Regression Techniques' is centered above a brief description: 'Predict sales prices and practice feature engineering, RFs, and gradient boosting'. Below this, it says '5,012 teams · Ongoing'. A navigation bar at the top includes 'Overview', 'Data', 'Kernels', 'Discussion', 'Leaderboard', 'Rules', 'Team', 'My Submissions', and a prominent blue 'Submit Predictions' button. The main content area has a sidebar on the left with links for 'Description', 'Evaluation', 'Frequently Asked Questions', and 'Tutorials'. The main panel starts with 'Start here if...' followed by a brief introduction for data science students. It then leads to the 'Competition Description' section.

Fig. 6.10.2: House Price Prediction

```
# If pandas is not installed, please uncomment the following line:
# !pip install pandas

%matplotlib inline
import d2l
from mxnet import autograd, gluon, init, nd
from mxnet.gluon import data as gdata, loss as gloss, nn
import numpy as np
import pandas as pd
```

For convenience, we already downloaded the data and stored it in the `../data` directory. To load the two CSV (Comma Separated Values) files containing training and test data respectively we use Pandas.

```
train_data = pd.read_csv('../data/kaggle_house_pred_train.csv')
test_data = pd.read_csv('../data/kaggle_house_pred_test.csv')
```

The training data set includes 1,460 examples, 80 features, and 1 label., the test data contains 1,459 examples and 80 features.

```
print(train_data.shape)
print(test_data.shape)
```

```
(1460, 81)
(1459, 80)
```

Let's take a look at the first 4 and last 2 features as well as the label (SalePrice) from the first 4 examples:

```
train_data.iloc[0:4, [0, 1, 2, 3, -3, -2, -1]]
```

We can see that in each example, the first feature is the ID. This helps the model identify each training example. While this is convenient, it doesn't carry any information for prediction purposes. Hence we remove it from the dataset before feeding the data into the network.

```
all_features = pd.concat((train_data.iloc[:, 1:-1], test_data.iloc[:, 1:]))
```

### 6.10.3 Data Preprocessing

As stated above, we have a wide variety of datatypes. Before we feed it into a deep network, we need to perform some amount of processing. Let's start with the numerical features. We begin by replacing missing values with the mean. This is a reasonable strategy if features are missing at random. To adjust them to a common scale, we rescale them to zero mean and unit variance. This is accomplished as follows:

$$x \leftarrow \frac{x - \mu}{\sigma} \quad (6.10.1)$$

To check that this transforms  $x$  to data with zero mean and unit variance simply calculate  $\mathbf{E}[(x - \mu)/\sigma] = (\mu - \mu)/\sigma = 0$ . To check the variance we use  $\mathbf{E}[(x - \mu)^2] = \sigma^2$  and thus the transformed variable has unit variance. The reason for ‘normalizing’ the data is that it brings all features to the same order of magnitude. After all, we do not know *a priori* which features are likely to be relevant.

```
numeric_features = all_features.dtypes[all_features.dtypes != 'object'].index
all_features[numeric_features] = all_features[numeric_features].apply(
    lambda x: (x - x.mean()) / (x.std()))
# After standardizing the data all means vanish, hence we can set missing
# values to 0
all_features[numeric_features] = all_features[numeric_features].fillna(0)
```

Next we deal with discrete values. This includes variables such as ‘MSZoning’. We replace them by a one-hot encoding in the same manner as how we transformed multiclass classification data into a vector of 0 and 1. For instance, ‘MSZoning’ assumes the values ‘RL’ and ‘RM’. They map into vectors  $(1, 0)$  and  $(0, 1)$  respectively. Pandas does this automatically for us.

```
# Dummy_na=True refers to a missing value being a legal eigenvalue, and
# creates an indicative feature for it
all_features = pd.get_dummies(all_features, dummy_na=True)
all_features.shape
```

```
(2919, 331)
```

You can see that this conversion increases the number of features from 79 to 331. Finally, via the `values` attribute, we can extract the NumPy format from the Pandas dataframe and convert it into MXNet's native NDArray representation for training.

```
n_train = train_data.shape[0]
train_features = nd.array(all_features[:n_train].values)
test_features = nd.array(all_features[n_train:].values)
train_labels = nd.array(train_data.SalePrice.values).reshape((-1, 1))
```

### 6.10.4 Training

To get started we train a linear model with squared loss. Not surprisingly, our linear model will not lead to a competition winning submission but it provides a sanity check to see whether there's meaningful information in the data. If we can't do better than random guessing here, then there might be a good chance that we have a data processing bug. And if things work, the linear model will serve as a baseline giving us some intuition about how close the simple model gets to the best reported models, giving us a sense of how much gain we should expect from fancier models.

```

loss = gloss.L2Loss()

def get_net():
    net = nn.Sequential()
    net.add(nn.Dense(1))
    net.initialize()
    return net

```

With house prices, as with stock prices, we care about relative quantities more than absolute quantities. More concretely, we tend to care more about the relative error  $\frac{y - \hat{y}}{y}$  than about the absolute error  $y - \hat{y}$ . For instance, if our prediction is off by USD 100,000 when estimating the price of a house in Rural Ohio, where the value of a typical house is 125,000 USD, then we are probably doing a horrible job. On the other hand, if we err by this amount in Los Altos Hills, California, this might represent a stunningly accurate prediction (their, the median house price exceeds 4 million USD).

One way to address this problem is to measure the discrepancy in the logarithm of the price estimates. In fact, this is also the official error metric used by the competition to measure the quality of submissions. After all, a small value  $\delta$  of  $\log y - \log \hat{y}$  translates into  $e^{-\delta} \leq \frac{\hat{y}}{y} \leq e^{\delta}$ . This leads to the following loss function:

$$L = \sqrt{\frac{1}{n} \sum_{i=1}^n (\log y_i - \log \hat{y}_i)^2} \quad (6.10.2)$$

```

def log_rmse(net, features, labels):
    # To further stabilize the value when the logarithm is taken, set the
    # value less than 1 as 1
    clipped_preds = nd.clip(net(features), 1, float('inf'))
    rmse = nd.sqrt(2 * loss(clipped_preds.log(), labels.log()).mean())
    return rmse.asscalar()

```

Unlike in previous sections, our training functions here will rely on the Adam optimizer (a slight variant on SGD that we will describe in greater detail later). The main appeal of Adam vs vanilla SGD is that the Adam optimizer, despite doing no better (and sometimes worse) given unlimited resources for hyperparameter optimization, people tend to find that it is significantly less sensitive to the initial learning rate. This will be covered in further detail later on when we discuss the details in [Section 12](#).

```

def train(net, train_features, train_labels, test_features, test_labels,
          num_epochs, learning_rate, weight_decay, batch_size):
    train_ls, test_ls = [], []
    train_iter = gdata.DataLoader(gdata.ArrayDataset(
        train_features, train_labels), batch_size, shuffle=True)
    # The Adam optimization algorithm is used here
    trainer = gluon.Trainer(net.collect_params(), 'adam', {
        'learning_rate': learning_rate, 'wd': weight_decay})
    for epoch in range(num_epochs):
        for X, y in train_iter:
            with autograd.record():
                l = loss(net(X), y)
                l.backward()
                trainer.step(batch_size)
            train_ls.append(log_rmse(net, train_features, train_labels))
        if test_labels is not None:

```

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```
    test_ls.append(log_rmse(net, test_features, test_labels))
return train_ls, test_ls
```

### 6.10.5 k-Fold Cross-Validation

If you are reading in a linear fashion, you might recall that we introduced k-fold cross-validation in the section where we discussed how to deal with model section (Section 6.4). We will put this to good use to select the model design and to adjust the hyperparameters. We first need a function that returns the i-th fold of the data in a k-fold cross-validation procedure. It proceeds by slicing out the i-th segment as validation data and returning the rest as training data. Note that this is not the most efficient way of handling data and we would definitely do something much smarter if our dataset was considerably larger. But this added complexity might obfuscate our code unnecessarily so we can safely omit here owing to the simplicity of our problem.

```
def get_k_fold_data(k, i, X, y):
    assert k > 1
    fold_size = X.shape[0] // k
    X_train, y_train = None, None
    for j in range(k):
        idx = slice(j * fold_size, (j + 1) * fold_size)
        X_part, y_part = X[idx, :], y[idx]
        if j == i:
            X_valid, y_valid = X_part, y_part
        elif X_train is None:
            X_train, y_train = X_part, y_part
        else:
            X_train = nd.concat(X_train, X_part, dim=0)
            y_train = nd.concat(y_train, y_part, dim=0)
    return X_train, y_train, X_valid, y_valid
```

The training and verification error averages are returned when we train  $k$  times in the k-fold cross-validation.

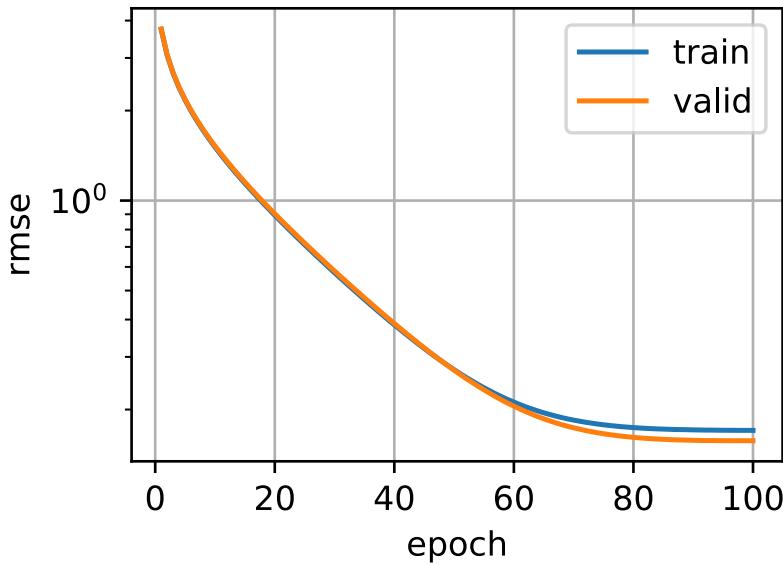
```
def k_fold(k, X_train, y_train, num_epochs,
          learning_rate, weight_decay, batch_size):
    train_l_sum, valid_l_sum = 0, 0
    for i in range(k):
        data = get_k_fold_data(k, i, X_train, y_train)
        net = get_net()
        train_ls, valid_ls = train(net, *data, num_epochs, learning_rate,
                                   weight_decay, batch_size)
        train_l_sum += train_ls[-1]
        valid_l_sum += valid_ls[-1]
        if i == 0:
            d2l.plot(list(range(1, num_epochs+1)), [train_ls, valid_ls],
                     xlabel='epoch', ylabel='rmse',
                     legend=['train', 'valid'], yscale='log')
        print('fold %d, train rmse: %f, valid rmse: %f' %
              (i, train_ls[-1], valid_ls[-1]))
    return train_l_sum / k, valid_l_sum / k
```

### 6.10.6 Model Selection

In this example, we pick an un-tuned set of hyperparameters and leave it up to the reader to improve the model. Finding a good choice can take quite some time, depending on how many things one wants to optimize over. Within reason, the k-fold cross-validation approach is resilient against multiple testing. However, if we were to try out an unreasonably large number of options it might fail since we might just get lucky on the validation split with a particular set of hyperparameters.

```
k, num_epochs, lr, weight_decay, batch_size = 5, 100, 5, 0, 64
train_l, valid_l = k_fold(k, train_features, train_labels, num_epochs, lr,
                         weight_decay, batch_size)
print('%d-fold validation: avg train rmse: %f, avg valid rmse: %f'
      % (k, train_l, valid_l))
```

```
fold 0, train rmse: 0.170321, valid rmse: 0.157338
fold 1, train rmse: 0.162391, valid rmse: 0.190203
fold 2, train rmse: 0.163539, valid rmse: 0.167801
fold 3, train rmse: 0.167654, valid rmse: 0.154628
fold 4, train rmse: 0.162152, valid rmse: 0.182555
5-fold validation: avg train rmse: 0.165212, avg valid rmse: 0.170505
```



You will notice that sometimes the number of training errors for a set of hyper-parameters can be very low, while the number of errors for the  $K$ -fold cross-validation may be higher. This is an indicator that we are overfitting. Therefore, when we reduce the amount of training errors, we need to check whether the amount of errors in the k-fold cross-validation have also been reduced accordingly.

### 6.10.7 Predict and Submit

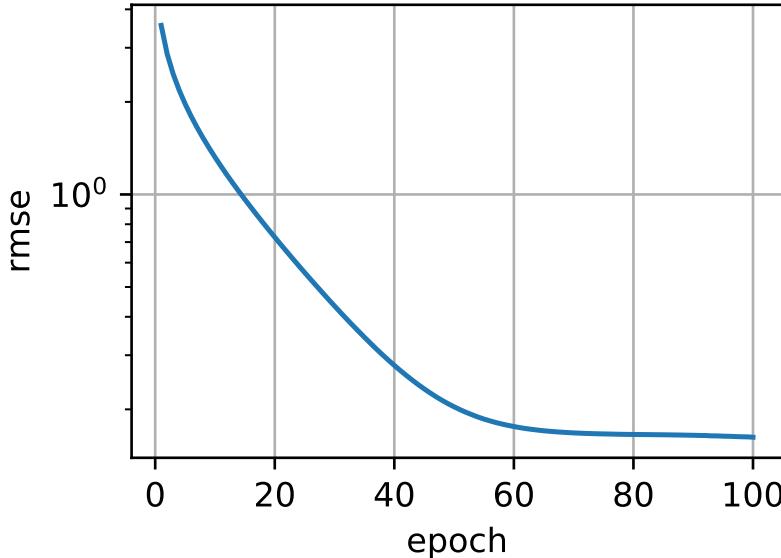
Now that we know what a good choice of hyperparameters should be, we might as well use all the data to train on it (rather than just  $1 - 1/k$  of the data that is used in the cross-validation slices). The model that we obtain in this way can then be applied to the test set. Saving the estimates in a CSV file will simplify uploading the results to Kaggle.

```
def train_and_pred(train_features, test_feature, train_labels, test_data,
                   num_epochs, lr, weight_decay, batch_size):
    net = get_net()
    train_ls, _ = train(net, train_features, train_labels, None, None,
                        num_epochs, lr, weight_decay, batch_size)
    d2l.plot(range(1, num_epochs+1), train_ls, xlabel='epoch', ylabel='rmse',
             yscale='log')
    print('train rmse %f' % train_ls[-1])
    # Apply the network to the test set
    preds = net(test_features).asnumpy()
    # Reformat it for export to Kaggle
    test_data['SalePrice'] = pd.Series(preds.reshape(1, -1)[0])
    submission = pd.concat([test_data['Id'], test_data['SalePrice']], axis=1)
    submission.to_csv('submission.csv', index=False)
```

Let's invoke our model. One nice sanity check is to see whether the predictions on the test set resemble those of the k-fold cross-validation process. If they do, it's time to upload them to Kaggle. The following code will generate a file called `submission.csv` (CSV is one of the file formats accepted by Kaggle):

```
train_and_pred(train_features, test_features, train_labels, test_data,
               num_epochs, lr, weight_decay, batch_size)
```

```
train rmse 0.162351
```



Next, we can submit our predictions on Kaggle and see how they compare to the actual house prices (labels) on the test set. The steps are quite simple:

- Log in to the Kaggle website and visit the House Price Prediction Competition page.
- Click the “Submit Predictions” or “Late Submission” button (as of this writing, the button is located on the right).
- Click the “Upload Submission File” button in the dashed box at the bottom of the page and select the prediction file you wish to upload.
- Click the “Make Submission” button at the bottom of the page to view your results.

The image shows a screenshot of the Kaggle submission interface. At the top left, it says "Step 1 Upload submission file". Below this is a dashed rectangular area containing an upward-pointing arrow icon and the text "Upload Submission File". To the right of this area, under "File Format", it says "Your submission should be in CSV format. You can upload this in a zip/gz/rar/7z archive, if you prefer." To the right of this, under "Number of Predictions", it says "We expect the solution file to have 1459 prediction rows. This file should have a header row. Please see sample submission file on the [data page](#)". At the bottom left, it says "Step 2 Describe submission". Below this is a rich text editor toolbar with icons for bold, italic, etc. To the right of the toolbar, it says "Styling with Markdown supported". Below the toolbar is a text input field with placeholder text "Briefly describe your submission." At the bottom center is a blue button labeled "Make Submission".

Fig. 6.10.3: Submitting data to Kaggle

### 6.10.8 Summary

- Real data often contains a mix of different datatypes and needs to be preprocessed.
- Rescaling real-valued data to zero mean and unit variance is a good default. So is replacing missing values with their mean.
- Transforming categorical variables into indicator variables allows us to treat them like vectors.
- We can use k-fold cross validation to select the model and adjust the hyper-parameters.
- Logarithms are useful for relative loss.

### 6.10.9 Exercises

1. Submit your predictions for this tutorial to Kaggle. How good are your predictions?
2. Can you improve your model by minimizing the log-price directly? What happens if you try to predict the log price rather than the price?
3. Is it always a good idea to replace missing values by their mean? Hint - can you construct a situation where the values are not missing at random?
4. Find a better representation to deal with missing values. Hint - What happens if you add an indicator variable?
5. Improve the score on Kaggle by tuning the hyperparameters through k-fold cross-validation.
6. Improve the score by improving the model (layers, regularization, dropout).

7. What happens if we do not standardize the continuous numerical features like we have done in this section?

#### 6.10.10 Scan the QR Code to Discuss<sup>91</sup>



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<sup>91</sup> <https://discuss.mxnet.io/t/2346>

## DEEP LEARNING COMPUTATION

Along side giant datasets and powerful hardware, great software tools have played an indispensable role in the rapid progress of deep learning. Starting with the pathbreaking Theano library released in 2007, flexible open-source tools have enabled researchers to rapidly prototype models avoiding repetitive work when recycling standard components while still maintaining the ability to make low-level modifications. Over time, deep learning's libraries have evolved to offer increasingly coarse abstractions. Just as semiconductor designers went from specifying transistors to logical circuits to writing code, neural networks researchers have moved from thinking about the behavior of individual artificial neurons to conceiving of networks in terms of whole layers, and now often design architectures with far coarser *blocks* in mind.

So far, we have introduced some basic machine learning concepts, ramping up to fully-functional deep learning models. In the last chapter, we implemented each component of a multilayer perceptron from scratch and even showed how to leverage MXNet's Gluon library to roll out the same models effortlessly. To get you that far that fast, we *called upon* the libraries, but skipped over more advanced details about *how they work*. In this chapter, we will peel back the curtain, digging deeper into the key components of deep learning computation, namely model construction, parameter access and initialization, designing custom layers and blocks, reading and writing models to disk, and leveraging GPUs to achieve dramatic speedups. These insights will move you from *end user* to *power user*, giving you the tools needed to combine the reap the benefits of a mature deep learning library, while retaining the flexibility to implement more complex models, including those you invent yourself! While this chapter does not introduce any new models or datasets, the advanced modeling chapters that follow rely heavily on these techniques.

### 7.1 Layers and Blocks

One of the key components that helped propel deep learning is powerful software. In an analogous manner to semiconductor design where engineers went from specifying transistors to logical circuits to writing code we now witness similar progress in the design of deep networks. The previous chapters have seen us move from designing single neurons to entire layers of neurons. However, even network design by layers can be tedious when we have 152 layers, as is the case in ResNet-152, which was proposed by He et al.<sup>92</sup> in 2016 for computer vision problems. Such networks have a fair degree of regularity and they consist of *blocks* of repeated (or at least similarly designed) layers. These blocks then form the basis of more complex network designs. In short, blocks are combinations of one or more layers. This design is aided by code that generates such blocks on demand, just like a Lego factory generates blocks which can be combined to produce terrific artifacts.

We start with very simple block, namely the block for a multilayer perceptron, such as the one we encountered in Section 6.3. A common strategy would be to construct a two-layer network as follows:

---

<sup>92</sup> [https://www.cv-foundation.org/openaccess/content\\_cvpr\\_2016/papers/He\\_Deep\\_Residual\\_Learning\\_CVPR\\_2016\\_paper.pdf](https://www.cv-foundation.org/openaccess/content_cvpr_2016/papers/He_Deep_Residual_Learning_CVPR_2016_paper.pdf)

```
from mxnet import nd
from mxnet.gluon import nn

x = nd.random.uniform(shape=(2, 20))

net = nn.Sequential()
net.add(nn.Dense(256, activation='relu'))
net.add(nn.Dense(10))
net.initialize()
net(x)
```

```
[[ 0.09543004  0.04614332 -0.00286654 -0.07790349 -0.05130243  0.02942037
  0.08696642 -0.0190793 -0.04122177  0.05088576]
 [ 0.0769287   0.03099705  0.00856576 -0.04467199 -0.06926839  0.09132434
  0.06786595 -0.06187842 -0.03436673  0.04234694]]
<NDArray 2x10 @cpu(0)>
```

This generates a network with a hidden layer of 256 units, followed by a ReLU activation and another 10 units governing the output. In particular, we used the `nn.Sequential` constructor to generate an empty network into which we then inserted both layers. What exactly happens inside `nn.Sequential` has remained rather mysterious so far. In the following we will see that this really just constructs a block. These blocks can be combined into larger artifacts, often recursively. The diagram below shows how:

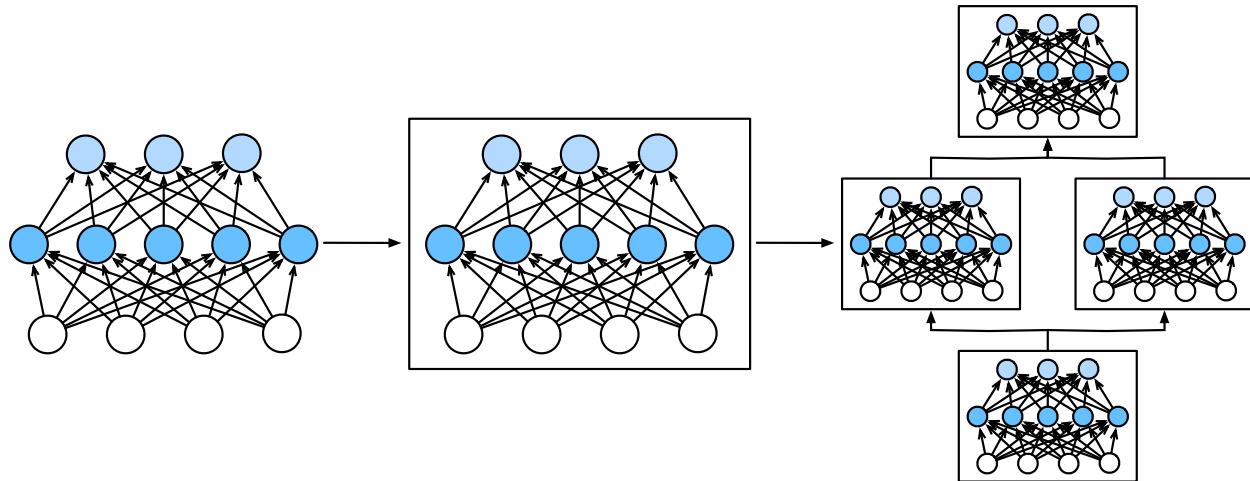


Fig. 7.1.1: Multiple layers are combined into blocks

In the following we will explain the various steps needed to go from defining layers to defining blocks (of one or more layers). To get started, we need a bit of reasoning about software. For most intents and purposes a block behaves very much like a fancy layer. That is, it provides the following functionality:

1. It needs to ingest data (the input).
2. It needs to produce a meaningful output. This is typically encoded in what we will call the `forward` function. It allows us to invoke a block via `net(X)` to obtain the desired output. What happens behind the scenes is that it invokes `forward` to perform forward propagation.
3. It needs to produce a gradient with regard to its input when invoking `backward`. Typically this is automatic.
4. It needs to store parameters that are inherent to the block. For instance, the block above contains two

hidden layers, and we need a place to store parameters for it.

- Obviously it also needs to initialize these parameters as needed.

### 7.1.1 A Custom Block

The `nn.Block` class provides the functionality required for much of what we need. It is a model constructor provided in the `nn` module, which we can inherit to define the model we want. The following inherits the `Block` class to construct the multilayer perceptron mentioned at the beginning of this section. The `MLP` class defined here overrides the `__init__` and `forward` functions of the `Block` class. They are used to create model parameters and define forward computations, respectively. Forward computation is also forward propagation.

```
from mxnet import nd
from mxnet.gluon import nn

class MLP(nn.Block):
    # Declare a layer with model parameters. Here, we declare two fully
    # connected layers
    def __init__(self, **kwargs):
        # Call the constructor of the MLP parent class Block to perform the
        # necessary initialization. In this way, other function parameters can
        # also be specified when constructing an instance, such as the model
        # parameter, params, described in the following sections
        super(MLP, self).__init__(**kwargs)
        self.hidden = nn.Dense(256, activation='relu') # Hidden layer
        self.output = nn.Dense(10) # Output layer

    # Define the forward computation of the model, that is, how to return the
    # required model output based on the input x
    def forward(self, x):
        return self.output(self.hidden(x))
```

Let's look at it a bit more closely. The `forward` method invokes a network simply by evaluating the hidden layer `self.hidden(x)` and subsequently by evaluating the output layer `self.output( ... )`. This is what we expect in the forward pass of this block.

In order for the block to know what it needs to evaluate, we first need to define the layers. This is what the `__init__` method does. It first initializes all of the `Block`-related parameters and then constructs the requisite layers. This attaches the corresponding layers and the required parameters to the class. Note that there is no need to define a backpropagation method in the class. The system automatically generates the `backward` method needed for back propagation by automatically finding the gradient. The same applies to the `initialize` method, which is generated automatically. Let's try this out:

```
net = MLP()
net.initialize()
net(x)
```

```
[[ 0.00362228  0.00633332  0.03201144 -0.01369375  0.10336449 -0.03508018
 -0.00032164 -0.01676023  0.06978628  0.01303309]
 [ 0.03871715  0.02608213  0.03544959 -0.02521311  0.11005433 -0.0143066
 -0.03052466 -0.03852827  0.06321152  0.0038594 ]]
<NDArray 2x10 @cpu(0)>
```

As explained above, the block class can be quite versatile in terms of what it does. For instance, its subclass

can be a layer (such as the `Dense` class provided by Gluon), it can be a model (such as the `MLP` class we just derived), or it can be a part of a model (this is what typically happens when designing very deep networks). Throughout this chapter we will see how to use this with great flexibility.

### 7.1.2 A Sequential Block

The `Block` class is a generic component describing dataflow. In fact, the `Sequential` class is derived from the `Block` class: when the forward computation of the model is a simple concatenation of computations for each layer, we can define the model in a much simpler way. The purpose of the `Sequential` class is to provide some useful convenience functions. In particular, the `add` method allows us to add concatenated `Block` subclass instances one by one, while the forward computation of the model is to compute these instances one by one in the order of addition. Below, we implement a `MySequential` class that has the same functionality as the `Sequential` class. This may help you understand more clearly how the `Sequential` class works.

```
class MySequential(nn.Block):
    def __init__(self, **kwargs):
        super(MySequential, self).__init__(**kwargs)

    def add(self, block):
        # Here, block is an instance of a Block subclass, and we assume it has
        # a unique name. We save it in the member variable _children of the
        # Block class, and its type is OrderedDict. When the MySequential
        # instance calls the initialize function, the system automatically
        # initializes all members of _children
        self._children[block.name] = block

    def forward(self, x):
        # OrderedDict guarantees that members will be traversed in the order
        # they were added
        for block in self._children.values():
            x = block(x)
        return x
```

At its core is the `add` method. It adds any block to the ordered dictionary of children. These are then executed in sequence when forward propagation is invoked. Let's see what the `MLP` looks like now.

```
net = MySequential()
net.add(nn.Dense(256, activation='relu'))
net.add(nn.Dense(10))
net.initialize()
net(x)
```

```
[[ 0.07787765  0.00216401  0.01682201  0.03059879 -0.00702019  0.01668714
   0.04822845  0.00394321 -0.09300036 -0.044943   ]
 [ 0.08891079 -0.00625484 -0.01619132  0.03807178 -0.01451489  0.02006172
   0.0303478   0.02463485 -0.07605445 -0.04389167]]
<NDArray 2x10 @cpu(0)>
```

Indeed, it can be observed that the use of the `MySequential` class is no different from the use of the `Sequential` class described in [Section 6.3](#).

### 7.1.3 Blocks with Code

Although the Sequential class can make model construction easier, and you do not need to define the `forward` method, directly inheriting the Block class can greatly expand the flexibility of model construction. In particular, we will use Python's control flow within the forward method. While we're at it, we need to introduce another concept, that of the `constant` parameter. These are parameters that are not used when invoking backprop. This sounds very abstract but here's what's really going on. Assume that we have some function

$$f(\mathbf{x}, \mathbf{w}) = 3 \cdot \mathbf{w}^\top \mathbf{x}. \quad (7.1.1)$$

In this case 3 is a constant parameter. We could change 3 to something else, say  $c$  via

$$f(\mathbf{x}, \mathbf{w}) = c \cdot \mathbf{w}^\top \mathbf{x}. \quad (7.1.2)$$

Nothing has really changed, except that we can adjust the value of  $c$ . It is still a constant as far as  $\mathbf{w}$  and  $\mathbf{x}$  are concerned. However, since Gluon doesn't know about this beforehand, it's worth while to give it a hand (this makes the code go faster, too, since we're not sending the Gluon engine on a wild goose chase after a parameter that doesn't change). `get_constant` is the method that can be used to accomplish this. Let's see what this looks like in practice.

```
class FancyMLP(nn.Block):
    def __init__(self, **kwargs):
        super(FancyMLP, self).__init__(**kwargs)
        # Random weight parameters created with the get_constant are not
        # iterated during training (i.e. constant parameters)
        self.rand_weight = self.params.get_constant(
            'rand_weight', nd.random.uniform(shape=(20, 20)))
        self.dense = nn.Dense(20, activation='relu')

    def forward(self, x):
        x = self.dense(x)
        # Use the constant parameters created, as well as the relu and dot
        # functions of NDArray
        x = nd.relu(nd.dot(x, self.rand_weight.data()) + 1)
        # Reuse the fully connected layer. This is equivalent to sharing
        # parameters with two fully connected layers
        x = self.dense(x)
        # Here in Control flow, we need to call asscalar to return the scalar
        # for comparison
        while x.norm().asscalar() > 1:
            x /= 2
        if x.norm().asscalar() < 0.8:
            x *= 10
        return x.sum()
```

In this FancyMLP model, we used constant weight `Rand_weight` (note that it is not a model parameter), performed a matrix multiplication operation (`nd.dot`), and reused the *same* `Dense` layer. Note that this is very different from using two dense layers with different sets of parameters. Instead, we used the same network twice. Quite often in deep networks one also says that the parameters are *tied* when one wants to express that multiple parts of a network share the same parameters. Let's see what happens if we construct it and feed data through it.

```
net = FancyMLP()  
net.initialize()  
net(x)
```

```
[25.522684]  
<NDArray 1 @cpu(0)>
```

There's no reason why we couldn't mix and match these ways of build a network. Obviously the example below resembles more a chimera, or less charitably, a [Rube Goldberg Machine](#)<sup>93</sup>. That said, it combines examples for building a block from individual blocks, which in turn, may be blocks themselves. Furthermore, we can even combine multiple strategies inside the same forward function. To demonstrate this, here's the network.

```
class NestMLP(nn.Block):
    def __init__(self, **kwargs):
        super(NestMLP, self).__init__(**kwargs)
        self.net = nn.Sequential()
        self.net.add(nn.Dense(64, activation='relu'),
                    nn.Dense(32, activation='relu'))
        self.dense = nn.Dense(16, activation='relu')

    def forward(self, x):
        return self.dense(self.net(x))

chimera = nn.Sequential()
chimera.add(NestMLP(), nn.Dense(20), FancyMLP())

chimera.initialize()
chimera(x)
```

[30.518448]

## 7.1.4 Compilation

The avid reader is probably starting to worry about the efficiency of this. After all, we have lots of dictionary lookups, code execution, and lots of other Pythonic things going on in what is supposed to be a high performance deep learning library. The problems of Python's [Global Interpreter Lock](#)<sup>94</sup> are well known. In the context of deep learning it means that we have a super fast GPU (or multiple of them) which might have to wait until a puny single CPU core running Python gets a chance to tell it what to do next. This is clearly awful and there are many ways around it. The best way to speed up Python is by avoiding it altogether.

Gluon does this by allowing for Hybridization ([Section 13.1](#)). In it, the Python interpreter executes the block the first time it's invoked. The Gluon runtime records what is happening and the next time around it short circuits any calls to Python. This can accelerate things considerably in some cases but care needs to be taken with control flow. We suggest that the interested reader skip forward to the section covering hybridization and compilation after finishing the current chapter.

<sup>93</sup> [https://en.wikipedia.org/wiki/Bube\\_Goldberg\\_machine](https://en.wikipedia.org/wiki/Bube_Goldberg_machine)

<sup>94</sup> <https://wiki.python.org/moin/GlobalInterpreterLock>

### 7.1.5 Summary

- Layers are blocks
- Many layers can be a block
- Many blocks can be a block
- Code can be a block
- Blocks take care of a lot of housekeeping, such as parameter initialization, backprop and related issues.
- Sequential concatenations of layers and blocks are handled by the eponymous `Sequential` block.

### 7.1.6 Exercises

1. What kind of error message will you get when calling an `__init__` method whose parent class not in the `__init__` function of the parent class?
2. What kinds of problems will occur if you remove the `asscalar` function in the `FancyMLP` class?
3. What kinds of problems will occur if you change `self.net` defined by the `Sequential` instance in the `NestMLP` class to `self.net = [nn.Dense(64, activation='relu'), nn.Dense(32, activation='relu')]`?
4. Implement a block that takes two blocks as an argument, say `net1` and `net2` and returns the concatenated output of both networks in the forward pass (this is also called a parallel block).
5. Assume that you want to concatenate multiple instances of the same network. Implement a factory function that generates multiple instances of the same block and build a larger network from it.

### 7.1.7 Scan the QR Code to Discuss<sup>95</sup>



## 7.2 Parameter Management

The ultimate goal of training deep networks is to find good parameter values for a given architecture. When everything is standard, the `nn.Sequential` class is a perfectly good tool for it. However, very few models are entirely standard and most scientists want to build things that are novel. This section shows how to manipulate parameters. In particular we will cover the following aspects:

- Accessing parameters for debugging, diagnostics, to visualize them or to save them is the first step to understanding how to work with custom models.
- Secondly, we want to set them in specific ways, e.g. for initialization purposes. We discuss the structure of parameter initializers.

<sup>95</sup> <https://discuss.mxnet.io/t/2325>

- Lastly, we show how this knowledge can be put to good use by building networks that share some parameters.

As always, we start from our trusty Multilayer Perceptron with a hidden layer. This will serve as our choice for demonstrating the various features.

```
from mxnet import init, nd
from mxnet.gluon import nn

net = nn.Sequential()
net.add(nn.Dense(256, activation='relu'))
net.add(nn.Dense(10))
net.initialize() # Use the default initialization method

x = nd.random.uniform(shape=(2, 20))
net(x) # Forward computation
```

```
[[ 0.09543004  0.04614332 -0.00286654 -0.07790349 -0.05130243  0.02942037
   0.08696642 -0.0190793  -0.04122177  0.05088576]
 [ 0.0769287   0.03099705  0.00856576 -0.04467199 -0.06926839  0.09132434
   0.06786595 -0.06187842 -0.03436673  0.04234694]]
<NDArray 2x10 @cpu(0)>
```

### 7.2.1 Parameter Access

In the case of a Sequential class we can access the parameters with ease, simply by indexing each of the layers in the network. The params variable then contains the required data. Let's try this out in practice by inspecting the parameters of the first layer.

```
print(net[0].params)
print(net[1].params)

dense0_ (
    Parameter dense0_weight (shape=(256, 20), dtype=float32)
    Parameter dense0_bias (shape=(256,), dtype=float32)
)
dense1_ (
    Parameter dense1_weight (shape=(10, 256), dtype=float32)
    Parameter dense1_bias (shape=(10,), dtype=float32)
)
```

The output tells us a number of things. Firstly, the layer consists of two sets of parameters: `dense0_weight` and `dense0_bias`, as we would expect. They are both single precision and they have the necessary shapes that we would expect from the first layer, given that the input dimension is 20 and the output dimension 256. In particular the names of the parameters are very useful since they allow us to identify parameters *uniquely* even in a network of hundreds of layers and with nontrivial structure. The second layer is structured accordingly.

#### Targeted Parameters

In order to do something useful with the parameters we need to access them, though. There are several ways to do this, ranging from simple to general. Let's look at some of them.

```
print(net[1].bias)
print(net[1].bias.data())
```

```
Parameter dense1_bias (shape=(10,), dtype=float32)

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
<NDArray 10 @cpu(0)>
```

The first returns the bias of the second layer. Since this is an object containing data, gradients, and additional information, we need to request the data explicitly. Note that the bias is all 0 since we initialized the bias to contain all zeros. Note that we can also access the parameters by name, such as `dense0_weight`. This is possible since each layer comes with its own parameter dictionary that can be accessed directly. Both methods are entirely equivalent but the first method leads to much more readable code.

```
print(net[0].params['dense0_weight'])
print(net[0].params['dense0_weight'].data())
```

```
Parameter dense0_weight (shape=(256, 20), dtype=float32)

[[ 0.06700657 -0.00369488  0.0418822 ... -0.05517294 -0.01194733
-0.00369594]
[-0.03296221 -0.04391347  0.03839272 ...  0.05636378  0.02545484
-0.007007 ]
[-0.0196689   0.01582889 -0.00881553 ...  0.01509629 -0.01908049
-0.02449339]
...
[ 0.00010955  0.0439323 -0.04911506 ...  0.06975312  0.0449558
-0.03283203]
[ 0.04106557  0.05671307 -0.00066976 ...  0.06387014 -0.01292654
0.00974177]
[ 0.00297424 -0.0281784 -0.06881659 ... -0.04047417  0.00457048
0.05696651]]
<NDArray 256x20 @cpu(0)>
```

Note that the weights are nonzero. This is by design since they were randomly initialized when we constructed the network. `data` is not the only function that we can invoke. For instance, we can compute the gradient with respect to the parameters. It has the same shape as the weight. However, since we did not invoke backpropagation yet, the values are all 0.

```
net[0].weight.grad()
```

```
[[0. 0. 0. ... 0. 0. 0.]
 [0. 0. 0. ... 0. 0. 0.]
 [0. 0. 0. ... 0. 0. 0.]
 ...
 [0. 0. 0. ... 0. 0. 0.]
 [0. 0. 0. ... 0. 0. 0.]
 [0. 0. 0. ... 0. 0. 0.]]
<NDArray 256x20 @cpu(0)>
```

## All Parameters at Once

Accessing parameters as described above can be a bit tedious, in particular if we have more complex blocks, or blocks of blocks (or even blocks of blocks of blocks), since we need to walk through the entire tree in reverse order to how the blocks were constructed. To avoid this, blocks come with a method `collect_params` which grabs all parameters of a network in one dictionary such that we can traverse it with ease. It does so by iterating over all constituents of a block and calls `collect_params` on subblocks as needed. To see the difference consider the following:

```
# parameters only for the first layer
print(net[0].collect_params())
# parameters of the entire network
print(net.collect_params())
```

```
dense0_ (
    Parameter dense0_weight (shape=(256, 20), dtype=float32)
    Parameter dense0_bias (shape=(256,), dtype=float32)
)
sequential0_ (
    Parameter dense0_weight (shape=(256, 20), dtype=float32)
    Parameter dense0_bias (shape=(256,), dtype=float32)
    Parameter dense1_weight (shape=(10, 256), dtype=float32)
    Parameter dense1_bias (shape=(10,), dtype=float32)
)
```

This provides us with a third way of accessing the parameters of the network. If we wanted to get the value of the bias term of the second layer we could simply use this:

```
net.collect_params()['dense1_bias'].data()
```

```
[0. 0. 0. 0. 0. 0. 0. 0. 0.]
<NDArray 10 @cpu(0)>
```

Throughout the book we'll see how various blocks name their subblocks (Sequential simply numbers them). This makes it very convenient to use regular expressions to filter out the required parameters.

```
print(net.collect_params('.*weight'))
print(net.collect_params('dense0.*'))

sequential0_ (
    Parameter dense0_weight (shape=(256, 20), dtype=float32)
    Parameter dense1_weight (shape=(10, 256), dtype=float32)
)
sequential0_ (
    Parameter dense0_weight (shape=(256, 20), dtype=float32)
    Parameter dense0_bias (shape=(256,), dtype=float32)
)
```

## Rube Goldberg strikes again

Let's see how the parameter naming conventions work if we nest multiple blocks inside each other. For that we first define a function that produces blocks (a block factory, so to speak) and then we combine these inside yet larger blocks.

```

def block1():
    net = nn.Sequential()
    net.add(nn.Dense(32, activation='relu'))
    net.add(nn.Dense(16, activation='relu'))
    return net

def block2():
    net = nn.Sequential()
    for i in range(4):
        net.add(block1())
    return net

rgnet = nn.Sequential()
rgnet.add(block2())
rgnet.add(nn.Dense(10))
rgnet.initialize()
rgnet(x)

```

```

[[ 1.0116727e-08 -9.4839003e-10 -1.1526797e-08  1.4917443e-08
  -1.5690811e-09 -3.9257650e-09 -4.1441655e-09  9.3013472e-09
   3.2393586e-09 -4.8612452e-09]
 [ 9.0111598e-09 -1.9115812e-10 -8.9595842e-09  1.0745880e-08
  1.4963460e-10 -2.2272872e-09 -3.9153973e-09  7.0595711e-09
   3.4854222e-09 -4.5807327e-09]]
<NDArray 2x10 @cpu(0)>

```

Now that we are done designing the network, let's see how it is organized. `collect_params` provides us with this information, both in terms of naming and in terms of logical structure.

```

print(rgnet.collect_params)
print(rgnet.collect_params())

```

```

<bound method Block.collect_params of Sequential(
 (0): Sequential(
 (0): Sequential(
 (0): Dense(20 -> 32, Activation(relu))
 (1): Dense(32 -> 16, Activation(relu))
 )
 (1): Sequential(
 (0): Dense(16 -> 32, Activation(relu))
 (1): Dense(32 -> 16, Activation(relu))
 )
 (2): Sequential(
 (0): Dense(16 -> 32, Activation(relu))
 (1): Dense(32 -> 16, Activation(relu))
 )
 (3): Sequential(
 (0): Dense(16 -> 32, Activation(relu))
 (1): Dense(32 -> 16, Activation(relu))
 )
 )
 (1): Dense(16 -> 10, linear)

```

(continues on next page)

(continued from previous page)

```
)>
sequential1_ (
    Parameter dense2_weight (shape=(32, 20), dtype=float32)
    Parameter dense2_bias (shape=(32,), dtype=float32)
    Parameter dense3_weight (shape=(16, 32), dtype=float32)
    Parameter dense3_bias (shape=(16,), dtype=float32)
    Parameter dense4_weight (shape=(32, 16), dtype=float32)
    Parameter dense4_bias (shape=(32,), dtype=float32)
    Parameter dense5_weight (shape=(16, 32), dtype=float32)
    Parameter dense5_bias (shape=(16,), dtype=float32)
    Parameter dense6_weight (shape=(32, 16), dtype=float32)
    Parameter dense6_bias (shape=(32,), dtype=float32)
    Parameter dense7_weight (shape=(16, 32), dtype=float32)
    Parameter dense7_bias (shape=(16,), dtype=float32)
    Parameter dense8_weight (shape=(32, 16), dtype=float32)
    Parameter dense8_bias (shape=(32,), dtype=float32)
    Parameter dense9_weight (shape=(16, 32), dtype=float32)
    Parameter dense9_bias (shape=(16,), dtype=float32)
    Parameter dense10_weight (shape=(10, 16), dtype=float32)
    Parameter dense10_bias (shape=(10,), dtype=float32)
)
```

Since the layers are hierarchically generated, we can also access them accordingly. For instance, to access the first major block, within it the second subblock and then within it, in turn the bias of the first layer, we perform the following.

```
rgnet[0][1][0].bias.data()
```

### 7.2.2 Parameter Initialization

Now that we know how to access the parameters, let's look at how to initialize them properly. We discussed the need for initialization in [Section 6.8](#). By default, MXNet initializes the weight matrices uniformly by drawing from  $U[-0.07, 0.07]$  and the bias parameters are all set to 0. However, we often need to use other methods to initialize the weights. MXNet's `init` module provides a variety of preset initialization methods, but if we want something out of the ordinary, we need a bit of extra work.

## Built-in Initialization

Let's begin with the built-in initializers. The code below initializes all parameters with Gaussian random variables.

```
# force_reinit ensures that the variables are initialized again, regardless of  
# whether they were already initialized previously  
net.initialize(init=init.Normal(sigma=0.01), force_reinit=True)  
net[0].weight.data()[0]
```

```
[ -0.008166 -0.00159167 -0.00273115  0.00684697  0.01204039  0.01359703
  0.00776908 -0.00640936  0.00256858  0.00545601  0.0018105 -0.00914027
  0.00133803  0.01070259 -0.00368285  0.01432678  0.00558631 -0.01479764
  0.00879013  0.00460165]
<NDArray 20 @cpu(0)>
```

If we wanted to initialize all parameters to 1, we could do this simply by changing the initializer to `Constant(1)`.

```
net.initialize(init=init.Constant(1), force_reinit=True)
net[0].weight.data() [0]
```

```
[1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.]
<NDArray 20 @cpu(0)>
```

If we want to initialize only a specific parameter in a different manner, we can simply set the initializer only for the appropriate subblock (or parameter) for that matter. For instance, below we initialize the second layer to a constant value of 42 and we use the `Xavier` initializer for the weights of the first layer.

```
net[1].initialize(init=init.Constant(42), force_reinit=True)
net[0].weight.initialize(init=init.Xavier(), force_reinit=True)
print(net[1].weight.data()[0,0])
print(net[0].weight.data()[0])
```

```
[42.]
<NDArray 1 @cpu(0)>

[-0.14511706 -0.01173057 -0.03754489 -0.14020921  0.00900492  0.01712246
 0.12447387 -0.04094418 -0.12105145  0.00079902 -0.0277361 -0.10213967
 -0.14027238 -0.02196661 -0.04641148  0.11977354  0.03604397 -0.14493202
 -0.06514931  0.13826048]
<NDArray 20 @cpu(0)>
```

## Custom Initialization

Sometimes, the initialization methods we need are not provided in the `init` module. At this point, we can implement a subclass of the `Initializer` class so that we can use it like any other initialization method. Usually, we only need to implement the `_init_weight` function and modify the incoming NDArray according to the initial result. In the example below, we pick a decidedly bizarre and nontrivial distribution, just to prove the point. We draw the coefficients from the following distribution:

$$w \sim \begin{cases} U[5, 10] & \text{with probability } \frac{1}{4} \\ 0 & \text{with probability } \frac{1}{2} \\ U[-10, -5] & \text{with probability } \frac{1}{4} \end{cases} \quad (7.2.1)$$

```
class MyInit(init.Initializer):
    def _init_weight(self, name, data):
        print('Init', name, data.shape)
        data[:] = nd.random.uniform(low=-10, high=10, shape=data.shape)
        data *= data.abs() >= 5
```

(continues on next page)

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```
net.initialize(MyInit(), force_reinit=True)
net[0].weight.data()[0]
```

```
Init dense0_weight (256, 20)
Init dense1_weight (10, 256)
```

```
[-5.44481   6.536484  -0.        0.        0.        7.7452965
 7.739216   7.6021366  0.        -0.       -7.3307705 -0.
 9.611603   0.        7.4357147  0.        0.        -0.
 8.446959   0.        ]
<NDArray 20 @cpu(0)>
```

If even this functionality is insufficient, we can set parameters directly. Since `data()` returns an NDArray we can access it just like any other matrix. A note for advanced users - if you want to adjust parameters within an `autograd` scope you need to use `set_data` to avoid confusing the automatic differentiation mechanics.

```
net[0].weight.data()[:] += 1
net[0].weight.data()[0,0] = 42
net[0].weight.data()[0]
```

```
[42.      7.536484  1.        1.        1.        8.7452965
 8.739216  8.602137  1.        1.       -6.3307705  1.
 10.611603 1.        8.435715  1.        1.        1.
 9.446959  1.        ]
<NDArray 20 @cpu(0)>
```

### 7.2.3 Tied Parameters

In some cases, we want to share model parameters across multiple layers. For instance when we want to find good word embeddings we may decide to use the same parameters both for encoding and decoding of words. We discussed one such case when we introduced [Section 7.1](#). Let's see how to do this a bit more elegantly. In the following we allocate a dense layer and then use its parameters specifically to set those of another layer.

```
net = nn.Sequential()
# We need to give the shared layer a name such that we can reference its
# parameters
shared = nn.Dense(8, activation='relu')
net.add(nn.Dense(8, activation='relu'),
       shared,
       nn.Dense(8, activation='relu', params=shared.params),
       nn.Dense(10))
net.initialize()

x = nd.random.uniform(shape=(2, 20))
net(x)

# Check whether the parameters are the same
print(net[1].weight.data()[0] == net[2].weight.data()[0])
```

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```
net[1].weight.data()[0,0] = 100
# Make sure that they're actually the same object rather than just having the
# same value
print(net[1].weight.data()[0] == net[2].weight.data()[0])
```

```
[1. 1. 1. 1. 1. 1. 1.]
<NDArray 8 @cpu(0)>

[1. 1. 1. 1. 1. 1. 1.]
<NDArray 8 @cpu(0)>
```

The above example shows that the parameters of the second and third layer are tied. They are identical rather than just being equal. That is, by changing one of the parameters the other one changes, too. What happens to the gradients is quite ingenious. Since the model parameters contain gradients, the gradients of the second hidden layer and the third hidden layer are accumulated in the `shared.params.grad()` during backpropagation.

## 7.2.4 Summary

- We have several ways to access, initialize, and tie model parameters.
- We can use custom initialization.
- Gluon has a sophisticated mechanism for accessing parameters in a unique and hierarchical manner.

## 7.2.5 Exercises

1. Use the FancyMLP defined in Section 7.1 and access the parameters of the various layers.
2. Look at the MXNet documentation<sup>96</sup> and explore different initializers.
3. Try accessing the model parameters after `net.initialize()` and before `net(x)` to observe the shape of the model parameters. What changes? Why?
4. Construct a multilayer perceptron containing a shared parameter layer and train it. During the training process, observe the model parameters and gradients of each layer.
5. Why is sharing parameters a good idea?

## 7.2.6 Scan the QR Code to Discuss<sup>97</sup>



<sup>96</sup> <http://beta.mxnet.io/api/gluon-related/mxnet.initializer.html>

<sup>97</sup> <https://discuss.mxnet.io/t/2326>

## 7.3 Deferred Initialization

In the previous examples we played fast and loose with setting up our networks. In particular we did the following things that *shouldn't* work:

- We defined the network architecture with no regard to the input dimensionality.
- We added layers without regard to the output dimension of the previous layer.
- We even ‘initialized’ these parameters without knowing how many parameters were to initialize.

All of those things sound impossible and indeed, they are. After all, there’s no way MXNet (or any other framework for that matter) could predict what the input dimensionality of a network would be. Later on, when working with convolutional networks and images this problem will become even more pertinent, since the input dimensionality (i.e. the resolution of an image) will affect the dimensionality of subsequent layers at a long range. Hence, the ability to set parameters without the need to know at the time of writing the code what the dimensionality is can greatly simplify statistical modeling. In what follows, we will discuss how this works using initialization as an example. After all, we cannot initialize variables that we don’t know exist.

### 7.3.1 Instantiating a Network

Let’s see what happens when we instantiate a network. We start with our trusty MLP as before.

```
from mxnet import init, nd
from mxnet.gluon import nn

def getnet():
    net = nn.Sequential()
    net.add(nn.Dense(256, activation='relu'))
    net.add(nn.Dense(10))
    return net

net = getnet()
```

At this point the network doesn’t really know yet what the dimensionalities of the various parameters should be. All one could tell at this point is that each layer needs weights and bias, albeit of unspecified dimensionality. If we try accessing the parameters, that’s exactly what happens.

```
print(net.collect_params)
print(net.collect_params())
```

```
<bound method Block.collect_params of Sequential(
  (0): Dense(None -> 256, Activation(relu))
  (1): Dense(None -> 10, linear)
)>
sequential0_ (
  Parameter dense0_weight (shape=(256, 0), dtype=float32)
  Parameter dense0_bias (shape=(256,), dtype=float32)
  Parameter dense1_weight (shape=(10, 0), dtype=float32)
  Parameter dense1_bias (shape=(10,), dtype=float32)
)
```

In particular, trying to access `net[0].weight.data()` at this point would trigger a runtime error stating that the network needs initializing before it can do anything. Let's see whether anything changes after we initialize the parameters:

```
net.initialize()
net.collect_params()
```

```
sequential0_ (
    Parameter dense0_weight (shape=(256, 0), dtype=float32)
    Parameter dense0_bias (shape=(256,), dtype=float32)
    Parameter dense1_weight (shape=(10, 0), dtype=float32)
    Parameter dense1_bias (shape=(10,), dtype=float32)
)
```

As we can see, nothing really changed. Only once we provide the network with some data, we see a difference. Let's try it out.

```
x = nd.random.uniform(shape=(2, 20))
net(x) # Forward computation

net.collect_params()
```

```
sequential0_ (
    Parameter dense0_weight (shape=(256, 20), dtype=float32)
    Parameter dense0_bias (shape=(256,), dtype=float32)
    Parameter dense1_weight (shape=(10, 256), dtype=float32)
    Parameter dense1_bias (shape=(10,), dtype=float32)
)
```

The main difference to before is that as soon as we knew the input dimensionality,  $\mathbf{x} \in \mathbb{R}^{20}$  it was possible to define the weight matrix for the first layer, i.e.  $\mathbf{W}_1 \in \mathbb{R}^{256 \times 20}$ . With that out of the way, we can progress to the second layer, define its dimensionality to be  $10 \times 256$  and so on through the computational graph and bind all the dimensions as they become available. Once this is known, we can proceed by initializing parameters. This is the solution to the three problems outlined above.

### 7.3.2 Deferred Initialization in Practice

Now that we know how it works in theory, let's see when the initialization is actually triggered. In order to do so, we mock up an initializer which does nothing but report a debug message stating when it was invoked and with which parameters.

```
class MyInit(init.Initializer):
    def __init_weight(self, name, data):
        print('Init', name, data.shape)
        # The actual initialization logic is omitted here

net = getnet()
net.initialize(init=MyInit())
```

Note that, although `MyInit` will print information about the model parameters when it is called, the above `initialize` function does not print any information after it has been executed. Therefore, there is no real parameter initialization when calling the `initialize` function. Next, we define the input and perform a forward calculation.

```
x = nd.random.uniform(shape=(2, 20))
y = net(x)
```

```
Init dense2_weight (256, 20)
Init dense3_weight (10, 256)
```

At this time, information on the model parameters is printed. When performing a forward calculation based on the input `x`, the system can automatically infer the shape of the weight parameters of all layers based on the shape of the input. Once the system has created these parameters, it calls the `MyInit` instance to initialize them before proceeding to the forward calculation.

Of course, this initialization will only be called when completing the initial forward calculation. After that, we will not re-initialize when we run the forward calculation `net(x)`, so the output of the `MyInit` instance will not be generated again.

```
y = net(x)
```

As mentioned at the beginning of this section, deferred initialization can also cause confusion. Before the first forward calculation, we were unable to directly manipulate the model parameters, for example, we could not use the `data` and `set_data` functions to get and modify the parameters. Therefore, we often force initialization by sending a sample observation through the network.

### 7.3.3 Forced Initialization

Deferred initialization does not occur if the system knows the shape of all parameters when calling the `initialize` function. This can occur in two cases:

- We've already seen some data and we just want to reset the parameters.
- We specified all input and output dimensions of the network when defining it.

The first case works just fine, as illustrated below.

```
net.initialize(init=MyInit(), force_reinit=True)
```

```
Init dense2_weight (256, 20)
Init dense3_weight (10, 256)
```

The second case requires us to specify the remaining set of parameters when creating the layer. For instance, for dense layers we also need to specify the `in_units` so that initialization can occur immediately once `initialize` is called.

```
net = nn.Sequential()
net.add(nn.Dense(256, in_units=20, activation='relu'))
net.add(nn.Dense(10, in_units=256))

net.initialize(init=MyInit())
```

```
Init dense4_weight (256, 20)
Init dense5_weight (10, 256)
```

### 7.3.4 Summary

- Deferred initialization is a good thing. It allows Gluon to set many things automagically and it removes a great source of errors from defining novel network architectures.
- We can override this by specifying all implicitly defined variables.
- Initialization can be repeated (or forced) by setting the `force_reinit=True` flag.

### 7.3.5 Exercises

1. What happens if you specify only parts of the input dimensions. Do you still get immediate initialization?
2. What happens if you specify mismatching dimensions?
3. What would you need to do if you have input of varying dimensionality? Hint - look at parameter tying.

### 7.3.6 Scan the QR Code to Discuss<sup>98</sup>



## 7.4 Custom Layers

One of the reasons for the success of deep learning can be found in the wide range of layers that can be used in a deep network. This allows for a tremendous degree of customization and adaptation. For instance, scientists have invented layers for images, text, pooling, loops, dynamic programming, even for computer programs. Sooner or later you will encounter a layer that doesn't exist yet in Gluon, or even better, you will eventually invent a new layer that works well for your problem at hand. This is when it's time to build a custom layer. This section shows you how.

### 7.4.1 Layers without Parameters

Since this is slightly intricate, we start with a custom layer (aka Block) that doesn't have any inherent parameters. Our first step is very similar to when we introduced blocks in Section 7.1. The following `CenteredLayer` class constructs a layer that subtracts the mean from the input. We build it by inheriting from the `Block` class and implementing the `forward` method.

```
from mxnet import gluon, nd
from mxnet.gluon import nn

class CenteredLayer(nn.Block):
    def __init__(self, **kwargs):
```

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<sup>98</sup> <https://discuss.mxnet.io/t/2327>

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```
super(CenteredLayer, self).__init__(**kwargs)

def forward(self, x):
    return x - x.mean()
```

To see how it works let's feed some data into the layer.

```
layer = CenteredLayer()
layer(nd.array([1, 2, 3, 4, 5]))
```

```
[ -2. -1.  0.  1.  2.]
<NDArray 5 @cpu(0)>
```

We can also use it to construct more complex models.

```
net = nn.Sequential()
net.add(nn.Dense(128), CenteredLayer())
net.initialize()
```

Let's see whether the centering layer did its job. For that we send random data through the network and check whether the mean vanishes. Note that since we're dealing with floating point numbers, we're going to see a very small albeit typically nonzero number.

```
y = net(nd.random.uniform(shape=(4, 8)))
y.mean().asscalar()
```

```
-7.212293e-10
```

## 7.4.2 Layers with Parameters

Now that we know how to define layers in principle, let's define layers with parameters. These can be adjusted through training. In order to simplify things for an avid deep learning researcher the `Parameter` class and the `ParameterDict` dictionary provide some basic housekeeping functionality. In particular, they govern access, initialization, sharing, saving and loading model parameters. For instance, this way we don't need to write custom serialization routines for each new custom layer.

For instance, we can use the member variable `params` of the `ParameterDict` type that comes with the `Block` class. It is a dictionary that maps string type parameter names to model parameters in the `Parameter` type. We can create a `Parameter` instance from `ParameterDict` via the `get` function.

```
params = gluon.ParameterDict()
params.get('param2', shape=(2, 3))
params
```

```
(
  Parameter param2 (shape=(2, 3), dtype=<class 'numpy.float32'>)
)
```

Let's use this to implement our own version of the dense layer. It has two parameters - bias and weight. To make it a bit nonstandard, we bake in the ReLU activation as default. Next, we implement a fully connected layer with both weight and bias parameters. It uses ReLU as an activation function, where `in_units` and `units` are the number of inputs and the number of outputs, respectively.

```

class MyDense(nn.Block):
    # units: the number of outputs in this layer; in_units: the number of
    # inputs in this layer
    def __init__(self, units, in_units, **kwargs):
        super(MyDense, self).__init__(**kwargs)
        self.weight = self.params.get('weight', shape=(in_units, units))
        self.bias = self.params.get('bias', shape=(units,))

    def forward(self, x):
        linear = nd.dot(x, self.weight.data()) + self.bias.data()
        return nd.relu(linear)

```

Naming the parameters allows us to access them by name through dictionary lookup later. It's a good idea to give them instructive names. Next, we instantiate the `MyDense` class and access its model parameters.

```

dense = MyDense(units=3, in_units=5)
dense.params

```

```

mydense0_(
    Parameter mydense0_weight (shape=(5, 3), dtype=<class 'numpy.float32'>)
    Parameter mydense0_bias (shape=(3,), dtype=<class 'numpy.float32'>)
)

```

We can directly carry out forward calculations using custom layers.

```

dense.initialize()
dense(nd.random.uniform(shape=(2, 5)))

```

```

[[0.06917784 0.01627153 0.01029644]
 [0.02602214 0.0453731 0.          ]]
<NDArray 2x3 @cpu(0)>

```

We can also construct models using custom layers. Once we have that we can use it just like the built-in dense layer. The only exception is that in our case size inference is not automagic. Please consult the [MXNet documentation](#)<sup>99</sup> for details on how to do this.

```

net = nn.Sequential()
net.add(MyDense(8, in_units=64),
       MyDense(1, in_units=8))
net.initialize()
net(nd.random.uniform(shape=(2, 64)))

```

```

[[0.03820474]
 [0.04035058]]
<NDArray 2x1 @cpu(0)>

```

### 7.4.3 Summary

- We can design custom layers via the `Block` class. This is more powerful than defining a block factory, since it can be invoked in many contexts.

<sup>99</sup> <http://www.mxnet.io>

- Blocks can have local parameters.

#### 7.4.4 Exercises

1. Design a layer that learns an affine transform of the data, i.e. it removes the mean and learns an additive parameter instead.
2. Design a layer that takes an input and computes a tensor reduction, i.e. it returns  $y_k = \sum_{i,j} W_{ijk} x_i x_j$ .
3. Design a layer that returns the leading half of the Fourier coefficients of the data. Hint - look up the `fft` function in MXNet.

#### 7.4.5 Scan the QR Code to Discuss<sup>100</sup>



### 7.5 File I/O

So far we discussed how to process data, how to build, train and test deep learning models. However, at some point we are likely happy with what we obtained and we want to save the results for later use and distribution. Likewise, when running a long training process it is best practice to save intermediate results (checkpointing) to ensure that we don't lose several days worth of computation when tripping over the power cord of our server. At the same time, we might want to load a pretrained model (e.g. we might have word embeddings for English and use it for our fancy spam classifier). For all of these cases we need to load and store both individual weight vectors and entire models. This section addresses both issues.

#### 7.5.1 NDArray

In its simplest form, we can directly use the `save` and `load` functions to store and read NDArrays separately. This works just as expected.

```
from mxnet import nd
from mxnet.gluon import nn

x = nd.arange(4)
nd.save('x-file', x)
```

Then, we read the data from the stored file back into memory.

```
x2 = nd.load('x-file')
x2
```

---

<sup>100</sup> <https://discuss.mxnet.io/t/2328>

```
[  
 [0. 1. 2. 3.]  
<NDArray 4 @cpu(0)>]
```

We can also store a list of NDArrays and read them back into memory.

```
y = nd.zeros(4)  
nd.save('x-files', [x, y])  
x2, y2 = nd.load('x-files')  
(x2, y2)
```

```
(  
 [0. 1. 2. 3.]  
<NDArray 4 @cpu(0)>,  
 [0. 0. 0. 0.]  
<NDArray 4 @cpu(0)>)
```

We can even write and read a dictionary that maps from a string to an NDArray. This is convenient, for instance when we want to read or write all the weights in a model.

```
mydict = {'x': x, 'y': y}  
nd.save('mydict', mydict)  
mydict2 = nd.load('mydict')  
mydict2
```

```
{'x':  
 [0. 1. 2. 3.]  
<NDArray 4 @cpu(0)>, 'y':  
 [0. 0. 0. 0.]  
<NDArray 4 @cpu(0)>}
```

## 7.5.2 Gluon Model Parameters

Saving individual weight vectors (or other NDArray tensors) is useful but it gets very tedious if we want to save (and later load) an entire model. After all, we might have hundreds of parameter groups sprinkled throughout. Writing a script that collects all the terms and matches them to an architecture is quite some work. For this reason Gluon provides built-in functionality to load and save entire networks rather than just single weight vectors. An important detail to note is that this saves model *parameters* and not the entire model. I.e. if we have a 3 layer MLP we need to specify the *architecture* separately. The reason for this is that the models themselves can contain arbitrary code, hence they cannot be serialized quite so easily (there is a way to do this for compiled models - please refer to the [MXNet documentation](#)<sup>101</sup> for the technical details on it). The result is that in order to reinstate a model we need to generate the architecture in code and then load the parameters from disk. The deferred initialization ([Section 7.3](#)) is quite advantageous here since we can simply define a model without the need to put actual values in place. Let's start with our favorite MLP.

```
class MLP(nn.Block):  
    def __init__(self, **kwargs):  
        super(MLP, self).__init__(**kwargs)  
        self.hidden = nn.Dense(256, activation='relu')
```

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<sup>101</sup> <http://www.mxnet.io>

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```
self.output = nn.Dense(10)

def forward(self, x):
    return self.output(self.hidden(x))

net = MLP()
net.initialize()
x = nd.random.uniform(shape=(2, 20))
y = net(x)
```

Next, we store the parameters of the model as a file with the name ‘mlp.params’.

```
net.save_parameters('mlp.params')
```

To check whether we are able to recover the model we instantiate a clone of the original MLP model. Unlike the random initialization of model parameters, here we read the parameters stored in the file directly.

```
clone = MLP()
clone.load_parameters('mlp.params')
```

Since both instances have the same model parameters, the computation result of the same input  $x$  should be the same. Let’s verify this.

```
yclone = clone(x)
yclone == y
```

```
[[1. 1. 1. 1. 1. 1. 1. 1. 1.]
 [1. 1. 1. 1. 1. 1. 1. 1. 1.]]
<NDArray 2x10 @cpu(0)>
```

### 7.5.3 Summary

- The `save` and `load` functions can be used to perform File I/O for NDArray objects.
- The `load_parameters` and `save_parameters` functions allow us to save entire sets of parameters for a network in Gluon.
- Saving the architecture has to be done in code rather than in parameters.

### 7.5.4 Exercises

1. Even if there is no need to deploy trained models to a different device, what are the practical benefits of storing model parameters?
2. Assume that we want to reuse only parts of a network to be incorporated into a network of a *different* architecture. How would you go about using, say the first two layers from a previous network in a new network.
3. How would you go about saving network architecture and parameters? What restrictions would you impose on the architecture?

### 7.5.5 Scan the QR Code to Discuss<sup>102</sup>



## 7.6 GPUs

In the introduction to this book we discussed the rapid growth of computation over the past two decades. In a nutshell, GPU performance has increased by a factor of 1000 every decade since 2000. This offers great opportunity but it also suggests a significant need to provide such performance.

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)

In this section we begin to discuss how to harness this compute performance for your research. First by using single GPUs and at a later point, how to use multiple GPUs and multiple servers (with multiple GPUs). You might have noticed that MXNet NDArray looks almost identical to NumPy. But there are a few crucial differences. One of the key features that differentiates MXNet from NumPy is its support for diverse hardware devices.

In MXNet, every array has a context. In fact, whenever we displayed an NDArray so far, it added a cryptic `@cpu(0)` notice to the output which remained unexplained so far. As we will discover, this just indicates that the computation is being executed on the CPU. Other contexts might be various GPUs. Things can get even hairier when we deploy jobs across multiple servers. By assigning arrays to contexts intelligently, we can minimize the time spent transferring data between devices. For example, when training neural networks on a server with a GPU, we typically prefer for the model's parameters to live on the GPU.

In short, for complex neural networks and large-scale data, using only CPUs for computation may be inefficient. In this section, we will discuss how to use a single NVIDIA GPU for calculations. First, make sure you have at least one NVIDIA GPU installed. Then, [download CUDA<sup>103</sup>](#) and follow the prompts to set the appropriate path. Once these preparations are complete, the `nvidia-smi` command can be used to view the graphics card information.

```
!nvidia-smi
```

```
Tue Jun 18 20:52:01 2019
```

```
+-----+
| NVIDIA-SMI 410.48           Driver Version: 410.48 |
+-----+
```

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<sup>102</sup> <https://discuss.mxnet.io/t/2329>

<sup>103</sup> <https://developer.nvidia.com/cuda-downloads>

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GPU	Name	Persistence-M	Bus-Id	Disp.A	Volatile	Uncorr.	ECC				
Fan	Temp	Perf	Pwr:Usage/Cap	Memory-Usage	GPU-Util	Compute M.					
<hr/>											
0	Tesla V100-SXM2...	On	00000000:00:1B.0	Off		0					
N/A	41C	P0	38W / 300W	0MiB / 16130MiB	0%	Default					
<hr/>											
1	Tesla V100-SXM2...	On	00000000:00:1C.0	Off		0					
N/A	40C	P0	38W / 300W	0MiB / 16130MiB	0%	Default					
<hr/>											
2	Tesla V100-SXM2...	On	00000000:00:1D.0	Off		0					
N/A	45C	P0	47W / 300W	0MiB / 16130MiB	0%	Default					
<hr/>											
3	Tesla V100-SXM2...	On	00000000:00:1E.0	Off		0					
N/A	42C	P0	41W / 300W	0MiB / 16130MiB	0%	Default					
<hr/>											
<hr/>											
Processes:											
GPU	PID	Type	Process name	GPU Memory							
<hr/>											
No running processes found											
<hr/>											

Next, we need to confirm that the GPU version of MXNet is installed. If a CPU version of MXNet is already installed, we need to uninstall it first. For example, use the `pip uninstall mxnet` command, then install the corresponding MXNet version according to the CUDA version. Assuming you have CUDA 9.0 installed, you can install the MXNet version that supports CUDA 9.0 by `pip install mxnet-cu90`. To run the programs in this section, you need at least two GPUs.

Note that this might be extravagant for most desktop computers but it is easily available in the cloud, e.g. by using the AWS EC2 multi-GPU instances. Almost all other sections do *not* require multiple GPUs. Instead, this is simply to illustrate how data flows between different devices.

### 7.6.1 Computing Devices

MXNet can specify devices, such as CPUs and GPUs, for storage and calculation. By default, MXNet creates data in the main memory and then uses the CPU to calculate it. In MXNet, the CPU and GPU can be indicated by `cpu()` and `gpu()`. It should be noted that `cpu()` (or any integer in the parentheses) means all physical CPUs and memory. This means that MXNet's calculations will try to use all CPU cores. However, `gpu()` only represents one graphic card and the corresponding graphic memory. If there are multiple GPUs, we use `gpu(i)` to represent the *i*-th GPU (*i* starts from 0). Also, `gpu(0)` and `gpu()` are equivalent.

```
from mxnet import nd, context
from mxnet.gluon import nn

context.cpu(), context.gpu(), context.gpu(1)

(cpu(0), gpu(0), gpu(1))
```

We can query the number of available GPUs through `num_gpus()`.

```
context.num_gpus()
```

```
2
```

Now we define two convenient functions that allows us to run codes even if the requested GPUs do not exist.

```
# Save to the d2l package.
def try_gpu(i=0):
    """Return gpu(i) if exists, otherwise return cpu()."""
    return context.gpu(i) if context.num_gpus() >= i + 1 else context.cpu()

# Save to the d2l package.
def try_all_gpus():
    """Return all available GPUs, or [cpu(),] if no GPU exists."""
    ctxes = [context.gpu(i) for i in range(context.num_gpus())]
    return ctxes if ctxes else [context.cpu()]

try_gpu(), try_gpu(3), try_all_gpus()
```

```
(gpu(0), cpu(0), [gpu(0), gpu(1)])
```

## 7.6.2 NDArray and GPUs

By default, NDArray objects are created on the CPU. Therefore, we will see the @cpu(0) identifier each time we print an NDArray.

```
x = nd.array([1, 2, 3])
x
```

```
[1. 2. 3.]
<NDArray 3 @cpu(0)>
```

We can use the `context` property of NDArray to view the device where the NDArray is located. It is important to note that whenever we want to operate on multiple terms they need to be in the same context. For instance, if we sum two variables, we need to make sure that both arguments are on the same device - otherwise MXNet would not know where to store the result or even how to decide where to perform the computation.

```
x.context
```

```
cpu(0)
```

### Storage on the GPU

There are several ways to store an NDArray on the GPU. For example, we can specify a storage device with the `ctx` parameter when creating an NDArray. Next, we create the NDArray variable `a` on `gpu(0)`. Notice that when printing `a`, the device information becomes `@gpu(0)`. The NDArray created on a GPU only consumes the memory of this GPU. We can use the `nvidia-smi` command to view GPU memory usage. In general, we need to make sure we do not create data that exceeds the GPU memory limit.

```
x = nd.ones((2, 3), ctx=try_gpu())
x
```

```
[[1. 1. 1.]
 [1. 1. 1.]]
<NDArray 2x3 @gpu(0)>
```

Assuming you have at least two GPUs, the following code will create a random array on `gpu(1)`.

```
y = nd.random.uniform(shape=(2, 3), ctx=try_gpu(1))
y
```

```
[[0.59119   0.313164   0.76352036]
 [0.9731786  0.35454726  0.11677533]]
<NDArray 2x3 @gpu(1)>
```

## Copying

If we want to compute  $\mathbf{x} + \mathbf{y}$  we need to decide where to perform this operation. For instance, we can transfer  $\mathbf{x}$  to `gpu(1)` and perform the operation there. **Do not** simply add  $\mathbf{x} + \mathbf{y}$  since this will result in an exception. The runtime engine wouldn't know what to do, it cannot find data on the same device and it fails.

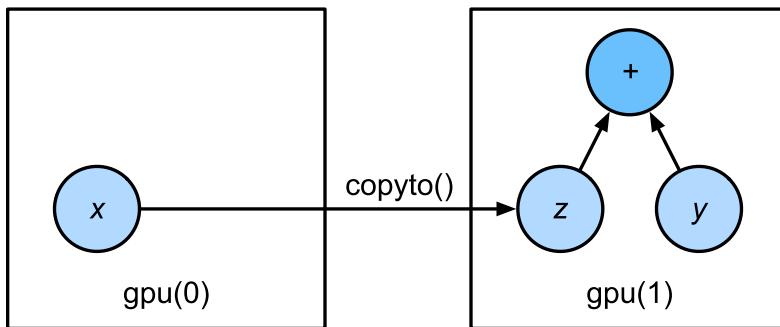


Fig. 7.6.1: Copyto copies arrays to the target device

`copyto` copies the data to another device such that we can add them. Since  $\mathbf{y}$  lives on the second GPU we need to move  $\mathbf{x}$  there before we can add the two.

```
z = x.copyto(try_gpu(1))
print(x)
print(z)
```

```
[[1. 1. 1.]
 [1. 1. 1.]]
<NDArray 2x3 @gpu(0)>

[[1. 1. 1.]
 [1. 1. 1.]]
<NDArray 2x3 @gpu(1)>
```

Now that the data is on the same GPU (both `z` and `y` are), we can add them up. In such cases MXNet places the result on the same device as its constituents. In our case that is `@gpu(1)`.

```
y + z
```

```
[[1.59119  1.313164  1.7635204]
 [1.9731786 1.3545473 1.1167753]]
<NDArray 2x3 @gpu(1)>
```

Imagine that your variable `z` already lives on your second GPU (`gpu(1)`). What happens if we call `z.copyto(gpu(1))`? It will make a copy and allocate new memory, even though that variable already lives on the desired device! There are times where depending on the environment our code is running in, two variables may already live on the same device. So we only want to make a copy if the variables currently lives on different contexts. In these cases, we can call `as_in_context()`. If the variable is already the specified context then this is a no-op. In fact, unless you specifically want to make a copy, `as_in_context()` is the method of choice.

```
z = x.as_in_context(try_gpu(1))
z
```

```
[[1. 1. 1.]
 [1. 1. 1.]]
<NDArray 2x3 @gpu(1)>
```

It is important to note that, if the `context` of the source variable and the target variable are consistent, then the `as_in_context` function causes the target variable and the source variable to share the memory of the source variable.

```
y.as_in_context(try_gpu(1)) is y
```

```
True
```

The `copyto` function always creates new memory for the target variable.

```
y.copyto(try_gpu(1)) is y
```

```
False
```

## Watch Out

People use GPUs to do machine learning because they expect them to be fast. But transferring variables between contexts is slow. So we want you to be 100% certain that you want to do something slow before we let you do it. If MXNet just did the copy automatically without crashing then you might not realize that you had written some slow code.

Also, transferring data between devices (CPU, GPUs, other machines) is something that is *much slower* than computation. It also makes parallelization a lot more difficult, since we have to wait for data to be sent (or rather to be received) before we can proceed with more operations. This is why copy operations should be taken with great care. As a rule of thumb, many small operations are much worse than one big operation. Moreover, several operations at a time are much better than many single operations interspersed in the code (unless you know what you're doing). This is the case since such operations can block if one device has to wait for the other before it can do something else. It's a bit like ordering your coffee in a queue rather than pre-ordering it by phone and finding out that it's ready when you are.

Lastly, when we print NDArray data or convert NDArrays to NumPy format, if the data is not in main memory, MXNet will copy it to the main memory first, resulting in additional transmission overhead. Even worse, it is now subject to the dreaded Global Interpreter Lock which makes everything wait for Python to complete.

### 7.6.3 Gluon and GPUs

Similar to NDArray, Gluon's model can specify devices through the `ctx` parameter during initialization. The following code initializes the model parameters on the GPU (we will see many more examples of how to run models on GPUs in the following, simply since they will become somewhat more compute intensive).

```
net = nn.Sequential()
net.add(nn.Dense(1))
net.initialize(ctx=try_gpu())
```

When the input is an NDArray on the GPU, Gluon will calculate the result on the same GPU.

```
net(x)
```

```
[[0.04995865]
 [0.04995865]
<NDArray 2x1 @gpu(0)>
```

Let us confirm that the model parameters are stored on the same GPU.

```
net[0].weight.data()
```

```
[[0.0068339  0.01299825  0.0301265 ]]
<NDArray 1x3 @gpu(0)>
```

In short, as long as all data and parameters are on the same device, we can learn models efficiently. In the following we will see several such examples.

### 7.6.4 Summary

- MXNet can specify devices for storage and calculation, such as CPU or GPU. By default, MXNet creates data in the main memory and then uses the CPU to calculate it.
- MXNet requires all input data for calculation to be **on the same device**, be it CPU or the same GPU.
- You can lose significant performance by moving data without care. A typical mistake is as follows: computing the loss for every minibatch on the GPU and reporting it back to the user on the commandline (or logging it in a NumPy array) will trigger a global interpreter lock which stalls all GPUs. It is much better to allocate memory for logging inside the GPU and only move larger logs.

### 7.6.5 Exercises

1. Try a larger computation task, such as the multiplication of large matrices, and see the difference in speed between the CPU and GPU. What about a task with a small amount of calculations?
2. How should we read and write model parameters on the GPU?

3. Measure the time it takes to compute 1000 matrix-matrix multiplications of  $100 \times 100$  matrices and log the matrix norm  $\text{tr}MM^\top$  one result at a time vs. keeping a log on the GPU and transferring only the final result.
4. Measure how much time it takes to perform two matrix-matrix multiplications on two GPUs at the same time vs. in sequence on one GPU (hint - you should see almost linear scaling).

#### 7.6.6 Scan the QR Code to Discuss<sup>104</sup>



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<sup>104</sup> <https://discuss.mxnet.io/t/2330>



## CONVOLUTIONAL NEURAL NETWORKS

In several of our previous examples, we have already come up against image data, which consist of pixels arranged in a 2D grid. Depending on whether we are looking at a black and white or color image, we might have either one or multiple numerical values corresponding to each pixel location. Until now, we have dealt with this rich structure in the least satisfying possible way. We simply threw away this spatial structure by flattening each image into a 1D vector, and fed it into a fully-connected network. These networks are invariant to the order of their inputs. We will get qualitatively identical results out of a multilayer perceptron whether we preserve the original order of our features or if we permute the columns of our design matrix before learning the parameters. Ideally, we would find a way to leverage our prior knowledge that nearby pixels are more related to each other.

In this chapter, we introduce convolutional neural networks (CNNs), a powerful family of neural networks that were designed for precisely this purpose. CNN-based network *architectures* now dominate the field of computer vision to such an extent that hardly anyone these days would develop a commercial application or enter a competition related to image recognition, object detection, or semantic segmentation, without basing their approach on them.

Modern ‘convnets’, as they are often called owe their design to inspirations from biology, group theory, and a healthy dose of experimental tinkering. In addition to their strong predictive performance, convolutional neural networks tend to be computationally efficient, both because they tend to require fewer parameters than dense architectures and also because convolutions are easy to parallelize across GPU cores. As a result, researchers have sought to apply convnets whenever possible, and increasingly they have emerged as credible competitors even on tasks with 1D sequence structure, such as audio, text, and time series analysis, where recurrent neural networks (introduced in the next chapter) are conventionally used. Some clever adaptations of CNNs have also brought them to bear on graph-structured data and in recommender systems.

First, we will walk through the basic operations that comprise the backbone of all modern convolutional networks. These include the convolutional layers themselves, nitty-gritty details including padding and stride, the pooling layers used to aggregate information across adjacent spatial regions, the use of multiple *channels* (also called *filters*) at each layer, and a careful discussion of the structure of modern architectures. We will conclude the chapter with a full working example of LeNet, the first convolutional network successfully deployed, long before the rise of modern deep learning. In the next chapter we’ll dive into full implementations of some of the recent popular neural networks whose designs are representative of most of the techniques commonly used to design modern convolutional neural networks.

### 8.1 From Dense Layers to Convolutions

The models that we’ve discussed so far are fine options if you’re dealing with *tabular* data. By *tabular* we mean that the data consists of rows corresponding to examples and columns corresponding to features. With tabular data, we might anticipate that pattern we seek could require modeling interactions among the features, but do not assume anything a priori about which features are related to each other or in what way.

Sometimes we truly may not have any knowledge to guide the construction of more cleverly-organized architectures. and in these cases, a multilayer perceptron is often the best that we can do. However, once we start dealing with high-dimensional perceptual data, these *structure-less* networks can grow unwieldy.

For instance, let's return to our running example of distinguishing cats from dogs. Say that we do a thorough job in data collection, collecting an annotated sets of high-quality 1-megapixel photographs. This means that the input into a network has *1 million dimensions*. Even an aggressive reduction to *1,000 hidden dimensions* would require a *dense* (fully-connected) layer to support  $10^9$  parameters. Unless we have an extremely large dataset (perhaps billions?), lots of GPUs, a talent for extreme distributed optimization, and an extraordinary amount of patience, learning the parameters of this network may turn out to be impossible.

A careful reader might object to this argument on the basis that 1 megapixel resolution may not be necessary. However, while you could get away with 100,000 pixels, we grossly underestimated the number of hidden nodes that it typically takes to learn good hidden representations of images. Learning a binary classifier with so many parameters might seem to require that we collect an enormous dataset, perhaps comparable to the number of dogs and cats on the planet. And yet both humans and computers are able to distinguish cats from dogs quite well, seemingly contradicting these conclusions. That's because images exhibit rich structure that is typically exploited by humans and machine learning models alike.

### 8.1.1 Invariances

Imagine that you want to detect an object in an image. It seems reasonable that whatever method we use to recognize objects should not be overly concerned with the precise *location* of the object shouldn't in the image. Ideally we could learn a system that would somehow exploit this knowledge. Pigs usually don't fly and planes usually don't swim. Nonetheless, we could still recognize a flying pig were one to appear. This idea is taken to an extreme in the children's game 'Where's Waldo', an example is shown in Fig. 8.1.1. The game consists of a number of chaotic scenes bursting with activity and Waldo shows up somewhere in each (typically lurking in some unlikely location). The reader's goal is to locate him. Despite his characteristic outfit, this can be surprisingly difficult, due to the large number of confounders.

Back to images, the intuitions we have been discussing could be made more concrete yielding a few key principles for building neural networks for computer vision:

1. Our vision systems should, in some sense, respond similarly to the same object regardless of where it appears in the image (Translation Invariance)
2. Our vision systems should, in some sense, focus on local regions, without regard for what else is happening in the image at greater distances. (Locality)

Let's see how this translates into mathematics.

### 8.1.2 Constraining the MLP

To start off let's consider what an MLP would look like with  $h \times w$  images as inputs (represented as matrices in math, and as 2D arrays in code), and hidden representations similarly organized as  $h \times w$  matrices / 2D arrays. Let  $x[i, j]$  and  $h[i, j]$  denote pixel location  $(i, j)$  in an image and hidden representation, respectively. Consequently, to have each of the  $hw$  hidden nodes receive input from each of the  $hw$  inputs, we would switch from using weight matrices (as we did previously in MLPs) to representing our parameters as four-dimensional weight tensors.

We could formally express this dense layer as follows:

$$h[i, j] = u[i, j] + \sum_{k, l} W[i, j, k, l] \cdot x[k, l] = u[i, j] + \sum_{a, b} V[i, j, a, b] \cdot x[i + a, j + b] \quad (8.1.1)$$

The switch from  $W$  to  $V$  is entirely cosmetic (for now) since there is a one-to-one correspondence between coefficients in both tensors. We simply re-index the subscripts  $(k, l)$  such that  $k = i + a$  and  $l = j + b$ . In



Fig. 8.1.1: Image via Walker Books

other words, we set  $V[i, j, a, b] = W[i, j, i + a, j + b]$ . The indices  $a, b$  run over both positive and negative offsets, covering the entire image. For any given location  $(i, j)$  in the hidden layer  $h[i, j]$ , we compute its value by summing over pixels in  $x$ , centered around  $(i, j)$  and weighted by  $V[i, j, a, b]$ .

Now let's invoke the first principle we established above—*translation invariance*. This implies that a shift in the inputs  $x$  should simply lead to a shift in the activations  $h$ . This is only possible if  $V$  and  $u$  don't actually depend on  $(i, j)$ , i.e., we have  $V[i, j, a, b] = V[a, b]$  and  $u$  is a constant. As a result we can simplify the definition for  $h$ .

$$h[i, j] = u + \sum_{a, b} V[a, b] \cdot x[i + a, j + b] \quad (8.1.2)$$

This is a convolution! We are effectively weighting pixels  $(i + a, j + b)$  in the vicinity of  $(i, j)$  with coefficients  $V[a, b]$  to obtain the value  $h[i, j]$ . Note that  $V[a, b]$  needs many fewer coefficients than  $V[i, j, a, b]$ . For a 1 megapixel image it has at most 1 million coefficients. This reduces the number of parameters by a factor of 1 million since it no longer depends on the location within the image. We have made significant progress!

Now let's invoke the second principle - *locality*. As motivated above, we believe that we shouldn't have to look very far away from  $(i, j)$  in order to glean relevant information to assess what is going on at  $h[i, j]$ . This means that outside some range  $|a|, |b| > \Delta$ , we should set  $V[a, b] = 0$ . Equivalently, we can rewrite  $h[i, j]$  as

$$h[i, j] = u + \sum_{a=-\Delta}^{\Delta} \sum_{b=-\Delta}^{\Delta} V[a, b] \cdot x[i + a, j + b] \quad (8.1.3)$$

This, in a nutshell is the convolutional layer. When the local region (also called a *receptive field*) is small, the difference as compared to a fully-connected network can be dramatic. While previously, we might have required billions of parameters to represent just a single layer in an image-processing network, we now typically need just a few hundred. The price that we pay for this drastic modification is that our features will be translation invariant and that our layer can only take local information into account. All learning depends on imposing inductive bias. When that bias agrees with reality, we get sample-efficient models that generalize well to unseen data. But of course, if those biases do not agree with reality, e.g. if images turned out not to be translation invariant,

### 8.1.3 Convolutions

Let's briefly review why the above operation is called a *convolution*. In mathematics, the convolution between two functions, say  $f, g : \mathbb{R}^d \rightarrow \mathbb{R}$  is defined as

$$[f * g](x) = \int_{\mathbb{R}^d} f(z)g(x - z)dz \quad (8.1.4)$$

That is, we measure the overlap between  $f$  and  $g$  when both functions are shifted by  $x$  and ‘flipped’. Whenever we have discrete objects, the integral turns into a sum. For instance, for vectors defined on  $\ell_2$ , i.e., the set of square summable infinite dimensional vectors with index running over  $\mathbb{Z}$  we obtain the following definition.

$$[f * g](i) = \sum_a f(a)g(i - a) \quad (8.1.5)$$

For two-dimensional arrays, we have a corresponding sum with indices  $(i, j)$  for  $f$  and  $(i - a, j - b)$  for  $g$  respectively. This looks similar to definition above, with one major difference. Rather than using  $(i + a, j + b)$ , we are using the difference instead. Note, though, that this distinction is mostly cosmetic since we can always match the notation by using  $\tilde{V}[a, b] = V[-a, -b]$  to obtain  $h = x * \tilde{V}$ . Also note that the original definition is actually a *cross correlation*. We will come back to this in the following section.

### 8.1.4 Waldo Revisited

Let's see what this looks like if we want to build an improved Waldo detector. The convolutional layer picks windows of a given size and weighs intensities according to the mask  $V$ . We expect that wherever the 'waldoness' is highest, we will also find a peak in the hidden layer activations.



Fig. 8.1.2: Find Waldo.

There's just a problem with this approach: so far we blissfully ignored that images consist of 3 channels: red, green and blue. In reality, images are quite two-dimensional objects but rather as a 3rd order tensor, e.g., with shape  $1024 \times 1024 \times 3$  pixels. Only two of these axes concern spatial relationships, while the 3rd can be regarded as assigning a multidimensional representation *to each pixel location*.

We thus index  $\mathbf{x}$  as  $x[i, j, k]$ . The convolutional mask has to adapt accordingly. Instead of  $V[a, b]$  we now have  $V[a, b, c]$ .

Moreover, just as our input consists of a 3rd order tensor it turns out to be a good idea to similarly formulate our hidden representations as 3rd order tensors. In other words, rather than just having a 1D representation corresponding to each spatial location, we want to have a multidimensional hidden representations corresponding to each spatial location. We could think of the hidden representation as comprising a number of 2D grids stacked on top of each other. These are sometimes called *channels* or *feature maps*. Intuitively you might imagine that at lower layers, some channels specialize to recognizing edges. We can take care of this by adding a fourth coordinate to  $V$  via  $V[a, b, c, d]$ . Putting all together we have:

$$h[i, j, k] = \sum_{a=-\Delta}^{\Delta} \sum_{b=-\Delta}^{\Delta} \sum_c V[a, b, c, k] \cdot x[i + a, j + b, c] \quad (8.1.6)$$

This is the definition of a convolutional neural network layer. There are still many operations that we need to address. For instance, we need to figure out how to combine all the activations to a single output (e.g. whether there's a Waldo in the image). We also need to decide how to compute things efficiently, how to combine multiple layers, and whether it is a good idea to have many narrow or a few wide layers. All of this will be addressed in the remainder of the chapter.

### 8.1.5 Summary

- Translation invariance in images implies that all patches of an image will be treated in the same manner.
- Locality means that only a small neighborhood of pixels will be used for computation.
- Channels on input and output allows for meaningful feature analysis.

### 8.1.6 Exercises

1. Assume that the size of the convolution mask is  $\Delta = 0$ . Show that in this case the convolutional mask implements an MLP independently for each set of channels.
2. Why might translation invariance not be a good idea after all? Does it make sense for pigs to fly?
3. What happens at the boundary of an image?
4. Derive an analogous convolutional layer for audio.
5. What goes wrong when you apply the above reasoning to text? Hint - what is the structure of language?
6. Prove that  $f \circledast g = g \circledast f$ .

### 8.1.7 Scan the QR Code to Discuss<sup>105</sup>



## 8.2 Convolutions for Images

Now that we understand how convolutional layers work in theory, we are ready to see how this works in practice. Since we have motivated convolutional neural networks by their applicability to image data, we will stick with image data in our examples, and begin by revisiting the convolutional layer that we introduced in the previous section. We note that strictly speaking, *convolutional* layers are a slight misnomer, since the operations are typically expressed as cross correlations.

### 8.2.1 The Cross-Correlation Operator

In a convolutional layer, an input array and a correlation kernel array are combined to produce an output array through a cross-correlation operation. Let's see how this works for two dimensions. In our example, the input is a two-dimensional array with a height of 3 and width of 3. We mark the shape of the array as  $3 \times 3$  or  $(3, 3)$ . The height and width of the kernel array are both 2. Common names for this array in the deep learning research community include *kernel* and *filter*. The shape of the kernel window (also known as the convolution window) is given precisely by the height and width of the kernel (here it is  $2 \times 2$ ).

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<sup>105</sup> <https://discuss.mxnet.io/t/2348>

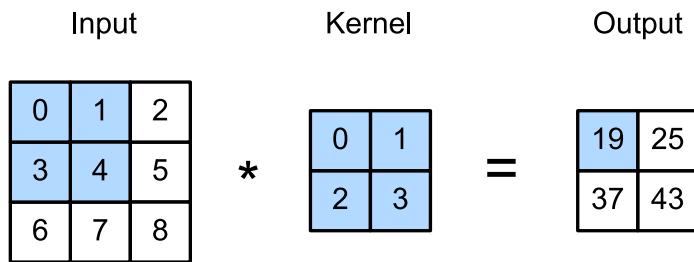


Fig. 8.2.1: Two-dimensional cross-correlation operation. The shaded portions are the first output element and the input and kernel array elements used in its computation:  $0 \times 0 + 1 \times 1 + 3 \times 2 + 4 \times 3 = 19$ .

In the two-dimensional cross-correlation operation, we begin with the convolution window positioned at the top-left corner of the input array and slide it across the input array, both from left to right and top to bottom. When the convolution window slides to a certain position, the input subarray contained in that window and the kernel array are multiplied (element-wise) and the resulting array is summed up yielding a single scalar value. This result is precisely the value of the output array at the corresponding location. Here, the output array has a height of 2 and width of 2 and the four elements are derived from the two-dimensional cross-correlation operation:

$$\begin{aligned}
 0 \times 0 + 1 \times 1 + 3 \times 2 + 4 \times 3 &= 19, \\
 1 \times 0 + 2 \times 1 + 4 \times 2 + 5 \times 3 &= 25, \\
 3 \times 0 + 4 \times 1 + 6 \times 2 + 7 \times 3 &= 37, \\
 4 \times 0 + 5 \times 1 + 7 \times 2 + 8 \times 3 &= 43.
 \end{aligned} \tag{8.2.1}$$

Note that along each axis, the output is slightly *smaller* than the input. Because the kernel has a width greater than one, and we can only compute the cross-correlation for locations where the kernel fits wholly within the image, the output size is given by the input size  $H \times W$  minus the size of the convolutional kernel  $h \times w$  via  $(H - h + 1) \times (W - w + 1)$ . This is the case since we need enough space to ‘shift’ the convolutional kernel across the image (later we will see how to keep the size unchanged by padding the image with zeros around its boundary such that there’s enough space to shift the kernel). Next, we implement the above process in the `corr2d` function. It accepts the input array `X` with the kernel array `K` and outputs the array `Y`.

```

from mxnet import autograd, nd
from mxnet.gluon import nn

# Save to the d2l package.
def corr2d(X, K):
    """Compute 2D cross-correlation."""
    h, w = K.shape
    Y = nd.zeros((X.shape[0] - h + 1, X.shape[1] - w + 1))
    for i in range(Y.shape[0]):
        for j in range(Y.shape[1]):
            Y[i, j] = (X[i:i + h, j:j + w] * K).sum()
    return Y

```

We can construct the input array `X` and the kernel array `K` from the figure above to validate the output of the above implementations of the two-dimensional cross-correlation operation.

```

X = nd.array([[0, 1, 2], [3, 4, 5], [6, 7, 8]])
K = nd.array([[0, 1], [2, 3]])
corr2d(X, K)

```

```
[[19. 25.]
 [37. 43.]]
<NDArray 2x2 @cpu(0)>
```

## 8.2.2 Convolutional Layers

A convolutional layer cross-correlates the input and kernels and adds a scalar bias to produce an output. The parameters of the convolutional layer are precisely the values that constitute the kernel and the scalar bias. When training the models based on convolutional layers, we typically initialize the kernels randomly, just as we would with a fully-connected layer.

We are now ready to implement a two-dimensional convolutional layer based on the `corr2d` function defined above. In the `__init__` constructor function, we declare `weight` and `bias` as the two model parameters. The forward computation function `forward` calls the `corr2d` function and adds the bias. As with  $h \times w$  cross-correlation we also refer to convolutional layers as  $h \times w$  convolutions.

```
class Conv2D(nn.Block):
    def __init__(self, kernel_size, **kwargs):
        super(Conv2D, self).__init__(**kwargs)
        self.weight = self.params.get('weight', shape=kernel_size)
        self.bias = self.params.get('bias', shape=(1,))

    def forward(self, x):
        return corr2d(x, self.weight.data()) + self.bias.data()
```

## 8.2.3 Object Edge Detection in Images

Let's look at a simple application of a convolutional layer: detecting the edge of an object in an image by finding the location of the pixel change. First, we construct an 'image' of  $6 \times 8$  pixels. The middle four columns are black (0) and the rest are white (1).

```
X = nd.ones((6, 8))
X[:, 2:6] = 0
X
```

```
[[1. 1. 0. 0. 0. 1. 1.]
 [1. 1. 0. 0. 0. 1. 1.]
 [1. 1. 0. 0. 0. 1. 1.]
 [1. 1. 0. 0. 0. 1. 1.]
 [1. 1. 0. 0. 0. 1. 1.]
 [1. 1. 0. 0. 0. 1. 1.]]
<NDArray 6x8 @cpu(0)>
```

Next, we construct a kernel  $K$  with a height of 1 and width of 2. When we perform the cross-correlation operation with the input, if the horizontally adjacent elements are the same, the output is 0. Otherwise, the output is non-zero.

```
K = nd.array([[1, -1]])
```

Enter  $X$  and our designed kernel  $K$  to perform the cross-correlation operations. As you can see, we will detect 1 for the edge from white to black and -1 for the edge from black to white. The rest of the outputs are 0.

```
Y = corr2d(X, K)
Y
```

```
[[ 0.  1.  0.  0.  0. -1.  0.]
 [ 0.  1.  0.  0.  0. -1.  0.]
 [ 0.  1.  0.  0.  0. -1.  0.]
 [ 0.  1.  0.  0.  0. -1.  0.]
 [ 0.  1.  0.  0.  0. -1.  0.]
 [ 0.  1.  0.  0.  0. -1.  0.]]
<NDArray 6x7 @cpu(0)>
```

Let's apply the kernel to the transposed image. As expected, it vanishes. The kernel K only detects vertical edges.

```
corr2d(X.T, K)
```

```
[[0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0.]]
<NDArray 8x5 @cpu(0)>
```

## 8.2.4 Learning a Kernel

Designing an edge detector by finite differences  $[1, -1]$  is neat if we know this is precisely what we are looking for. However, as we look at larger kernels, and consider successive layers of convolutions, it might be impossible to specify precisely what each filter should be doing manually.

Now let's see whether we can learn the kernel that generated Y from X by looking at the (input, output) pairs only. We first construct a convolutional layer and initialize its kernel as a random array. Next, in each iteration, we will use the squared error to compare Y and the output of the convolutional layer, then calculate the gradient to update the weight. For the sake of simplicity, in this convolutional layer, we will ignore the bias.

We previously constructed the `Conv2D` class. However, since we used single-element assignments, Gluon has some trouble finding the gradient. Instead, we use the built-in `Conv2D` class provided by Gluon below.

```
# Construct a convolutional layer with 1 output channel
# (channels will be introduced in the following section)
# and a kernel array shape of (1, 2)
conv2d = nn.Conv2D(1, kernel_size=(1, 2))
conv2d.initialize()

# The two-dimensional convolutional layer uses four-dimensional input and
# output in the format of (example, channel, height, width), where the batch
# size (number of examples in the batch) and the number of channels are both 1
X = X.reshape((1, 1, 6, 8))
Y = Y.reshape((1, 1, 6, 7))
```

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```

for i in range(10):
    with autograd.record():
        Y_hat = conv2d(X)
        l = (Y_hat - Y) ** 2
    l.backward()
    # For the sake of simplicity, we ignore the bias here
    conv2d.weight.data[:] -= 3e-2 * conv2d.weight.grad()
    if (i + 1) % 2 == 0:
        print('batch %d, loss %.3f' % (i + 1, l.sum().asscalar()))

```

```

batch 2, loss 4.949
batch 4, loss 0.831
batch 6, loss 0.140
batch 8, loss 0.024
batch 10, loss 0.004

```

As you can see, the error has dropped to a small value after 10 iterations. Now we will take a look at the kernel array we learned.

```
conv2d.weight.data().reshape((1, 2))
```

```

[[ 0.9895 -0.9873705]]
<NDArray 1x2 @cpu(0)>

```

Indeed, the learned kernel array is remarkably close to the kernel array  $K$  we defined earlier.

### 8.2.5 Cross-correlation and Convolution

Recall the observation from the previous section that cross-correlation and convolution are equivalent. In the figure above it is easy to see this correspondence. Simply flip the kernel from the bottom left to the top right. In this case the indexing in the sum is reverted, yet the same result can be obtained. In keeping with standard terminology with deep learning literature, we will continue to refer to the cross-correlation operation as a convolution even though, strictly-speaking, it is slightly different.

### 8.2.6 Summary

- The core computation of a two-dimensional convolutional layer is a two-dimensional cross-correlation operation. In its simplest form, this performs a cross-correlation operation on the two-dimensional input data and the kernel, and then adds a bias.
- We can design a kernel to detect edges in images.
- We can learn the kernel through data.

### 8.2.7 Exercises

1. Construct an image  $X$  with diagonal edges.
  - What happens if you apply the kernel  $K$  to it?
  - What happens if you transpose  $X$ ?

- What happens if you transpose K?
2. When you try to automatically find the gradient for the Conv2D class we created, what kind of error message do you see?
  3. How do you represent a cross-correlation operation as a matrix multiplication by changing the input and kernel arrays?
  4. Design some kernels manually.
    - What is the form of a kernel for the second derivative?
    - What is the kernel for the Laplace operator?
    - What is the kernel for an integral?
    - What is the minimum size of a kernel to obtain a derivative of degree  $d$ ?

#### 8.2.8 Scan the QR Code to Discuss<sup>106</sup>



### 8.3 Padding and Stride

In the previous example, our input had a height and width of 3 and a convolution kernel with a height and width of 2, yielding an output with a height and a width of 2. In general, assuming the input shape is  $n_h \times n_w$  and the convolution kernel window shape is  $k_h \times k_w$ , then the output shape will be

$$(n_h - k_h + 1) \times (n_w - k_w + 1). \quad (8.3.1)$$

Therefore, the output shape of the convolutional layer is determined by the shape of the input and the shape of the convolution kernel window.

In several cases we might want to incorporate particular techniques—padding and strides—regarding the size of the output:

- In general, since kernels generally have width and height greater than 1, that means that after applying many successive convolutions, we will wind up with an output that is much smaller than our input. If we start with a 240x240 pixel image, 10 layers of 5x5 convolutions reduce the image to 200x200 pixels, slicing off 30% of the image and with it obliterating any interesting information on the boundaries of the original image. *Padding* handles this issue.
- In some cases, we want to reduce the resolution drastically if say we find our original input resolution to be unwieldy. *Strides* can help in these instances.

---

<sup>106</sup> <https://discuss.mxnet.io/t/2349>

### 8.3.1 Padding

As described above, one tricky issue when applying convolutional layers is that losing pixels on the perimeter of our image. Since we typically use small kernels, for any given convolution, we might only lose a few pixels, but this can add up as we apply many successive convolutional layers. One straightforward solution to this problem is to add extra pixels of filler around the boundary of our input image, thus increasing the effective size of the image. Typically, we set the values of the extra pixels to 0. In the figure below, we pad a  $3 \times 3$  input, increasing its size to  $5 \times 5$ . The corresponding output then increases to a  $4 \times 4$  matrix.

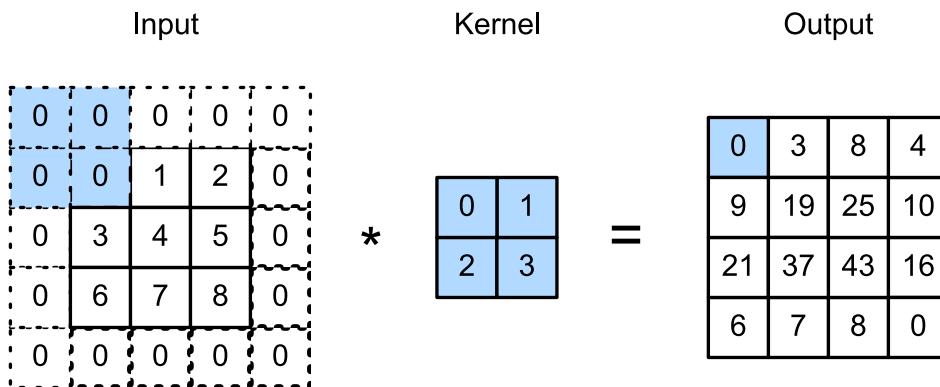


Fig. 8.3.1: Two-dimensional cross-correlation with padding. The shaded portions are the input and kernel array elements used by the first output element:  $0 \times 0 + 0 \times 1 + 0 \times 2 + 0 \times 3 = 0$ .

In general, if we add a total of  $p_h$  rows of padding (roughly half on top and half on bottom) and a total of  $p_w$  columns of padding (roughly half on the left and half on the right), the output shape will be

$$(n_h - k_h + p_h + 1) \times (n_w - k_w + p_w + 1), \quad (8.3.2)$$

This means that the height and width of the output will increase by  $p_h$  and  $p_w$  respectively.

In many cases, we will want to set  $p_h = k_h - 1$  and  $p_w = k_w - 1$  to give the input and output the same height and width. This will make it easier to predict the output shape of each layer when constructing the network. Assuming that  $k_h$  is odd here, we will pad  $p_h/2$  rows on both sides of the height. If  $k_h$  is even, one possibility is to pad  $\lceil p_h/2 \rceil$  rows on the top of the input and  $\lfloor p_h/2 \rfloor$  rows on the bottom. We will pad both sides of the width in the same way.

Convolutional neural networks commonly use convolutional kernels with odd height and width values, such as 1, 3, 5, or 7. Choosing odd kernel sizes has the benefit that we can preserve the spatial dimensionality while padding with the same number of rows on top and bottom, and the same number of columns on left and right.

Moreover, this practice of using odd kernels and padding to precisely preserve dimensionality offers a clerical benefit. For any two-dimensional array  $X$ , when the kernels size is odd and the number of padding rows and columns on all sides are the same, producing an output with the same height and width as the input, we know that the output  $Y[i, j]$  is calculated by cross-correlation of the input and convolution kernel with the window centered on  $X[i, j]$ .

In the following example, we create a two-dimensional convolutional layer with a height and width of 3 and apply 1 pixel of padding on all sides. Given an input with a height and width of 8, we find that the height and width of the output is also 8.

```
from mxnet import nd
from mxnet.gluon import nn
```

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```
# For convenience, we define a function to calculate the convolutional layer.
# This function initializes the convolutional layer weights and performs
# corresponding dimensionality elevations and reductions on the input and
# output
def comp_conv2d(conv2d, X):
    conv2d.initialize()
    # (1,1) indicates that the batch size and the number of channels
    # (described in later chapters) are both 1
    X = X.reshape((1, 1) + X.shape)
    Y = conv2d(X)
    # Exclude the first two dimensions that do not interest us: batch and
    # channel
    return Y.reshape(Y.shape[2:])

# Note that here 1 row or column is padded on either side, so a total of 2
# rows or columns are added
conv2d = nn.Conv2D(1, kernel_size=3, padding=1)
X = nd.random.uniform(shape=(8, 8))
comp_conv2d(conv2d, X).shape
```

(8, 8)

When the height and width of the convolution kernel are different, we can make the output and input have the same height and width by setting different padding numbers for height and width.

```
# Here, we use a convolution kernel with a height of 5 and a width of 3. The
# padding numbers on both sides of the height and width are 2 and 1,
# respectively
conv2d = nn.Conv2D(1, kernel_size=(5, 3), padding=(2, 1))
comp_conv2d(conv2d, X).shape
```

(8, 8)

### 8.3.2 Stride

When computing the cross-correlation, we start with the convolution window at the top-left corner of the input array, and then slide it over all locations both down and to the right. In previous examples, we default to sliding one pixel at a time. However, sometimes, either for computational efficiency or because we wish to downsample, we move our window more than one pixel at a time, skipping the intermediate locations.

We refer to the number of rows and columns traversed per slide as the *stride*. So far, we have used strides of 1, both for height and width. Sometimes, we may want to use a larger stride. The figure below shows a two-dimensional cross-correlation operation with a stride of 3 vertically and 2 horizontally. We can see that when the second element of the first column is output, the convolution window slides down three rows. The convolution window slides two columns to the right when the second element of the first row is output. When the convolution window slides two columns to the right on the input, there is no output because the input element cannot fill the window (unless we add padding).

In general, when the stride for the height is  $s_h$  and the stride for the width is  $s_w$ , the output shape is

$$\lfloor (n_h - k_h + p_h + s_h)/s_h \rfloor \times \lfloor (n_w - k_w + p_w + s_w)/s_w \rfloor. \quad (8.3.3)$$

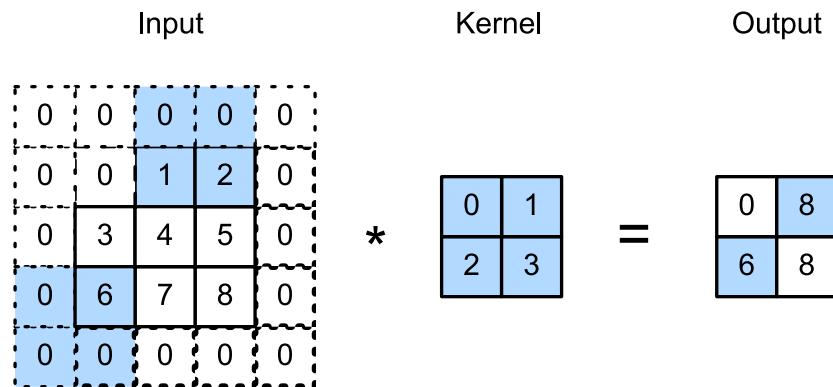


Fig. 8.3.2: Cross-correlation with strides of 3 and 2 for height and width respectively. The shaded portions are the output element and the input and core array elements used in its computation:  $0 \times 0 + 0 \times 1 + 1 \times 2 + 2 \times 3 = 8$ ,  $0 \times 0 + 6 \times 1 + 0 \times 2 + 0 \times 3 = 6$ .

If we set  $p_h = k_h - 1$  and  $p_w = k_w - 1$ , then the output shape will be simplified to  $\lfloor (n_h + s_h - 1)/s_h \rfloor \times \lfloor (n_w + s_w - 1)/s_w \rfloor$ . Going a step further, if the input height and width are divisible by the strides on the height and width, then the output shape will be  $(n_h/s_h) \times (n_w/s_w)$ .

Below, we set the strides on both the height and width to 2, thus halving the input height and width.

```
conv2d = nn.Conv2D(1, kernel_size=3, padding=1, strides=2)
comp_conv2d(conv2d, X).shape
```

```
(4, 4)
```

Next, we will look at a slightly more complicated example.

```
conv2d = nn.Conv2D(1, kernel_size=(3, 5), padding=(0, 1), strides=(3, 4))
comp_conv2d(conv2d, X).shape
```

```
(2, 2)
```

For the sake of brevity, when the padding number on both sides of the input height and width are  $p_h$  and  $p_w$  respectively, we call the padding  $(p_h, p_w)$ . Specifically, when  $p_h = p_w = p$ , the padding is  $p$ . When the strides on the height and width are  $s_h$  and  $s_w$ , respectively, we call the stride  $(s_h, s_w)$ . Specifically, when  $s_h = s_w = s$ , the stride is  $s$ . By default, the padding is 0 and the stride is 1. In practice we rarely use inhomogeneous strides or padding, i.e., we usually have  $p_h = p_w$  and  $s_h = s_w$ .

### 8.3.3 Summary

- Padding can increase the height and width of the output. This is often used to give the output the same height and width as the input.
- The stride can reduce the resolution of the output, for example reducing the height and width of the output to only  $1/n$  of the height and width of the input ( $n$  is an integer greater than 1).
- Padding and stride can be used to adjust the dimensionality of the data effectively.

### 8.3.4 Exercises

1. For the last example in this section, use the shape calculation formula to calculate the output shape to see if it is consistent with the experimental results.
2. Try other padding and stride combinations on the experiments in this section.
3. For audio signals, what does a stride of 2 correspond to?
4. What are the computational benefits of a stride larger than 1.

### 8.3.5 Scan the QR Code to Discuss<sup>107</sup>



## 8.4 Multiple Input and Output Channels

While we have described the multiple channels that comprise each image (e.g. color images have the standard RGB channels to indicate the amount of red, green and blue), until now, we simplified all of our numerical examples by working with just a single input and a single output channel. This has allowed us to think of our inputs, convolutional kernels, and outputs each as two-dimensional arrays.

When we add channels into the mix, our inputs and hidden representations both become three-dimensional arrays. For example, each RGB input image has shape  $3 \times h \times w$ . We refer to this axis, with a size of 3, as the channel dimension. In this section, we will take a deeper look at convolution kernels with multiple input and multiple output channels.

### 8.4.1 Multiple Input Channels

When the input data contains multiple channels, we need to construct a convolution kernel with the same number of input channels as the input data, so that it can perform cross-correlation with the input data. Assuming that the number of channels for the input data is  $c_i$ , the number of input channels of the convolution kernel also needs to be  $c_i$ . If our convolution kernel's window shape is  $k_h \times k_w$ , then when  $c_i = 1$ , we can think of our convolution kernel as just a two-dimensional array of shape  $k_h \times k_w$ .

However, when  $c_i > 1$ , we need a kernel that contains an array of shape  $k_h \times k_w$  for each input channel. Concatenating these  $c_i$  arrays together yields a convolution kernel of shape  $c_i \times k_h \times k_w$ . Since the input and convolution kernel each have  $c_i$  channels, we can perform a cross-correlation operation on the two-dimensional array of the input and the two-dimensional kernel array of the convolution kernel for each channel, adding the  $c_i$  results together (summing over the channels) to yield a two-dimensional array. This is the result of a two-dimensional cross-correlation between multi-channel input data and a *multi-input channel* convolution kernel.

In the figure below, we demonstrate an example of a two-dimensional cross-correlation with two input channels. The shaded portions are the first output element as well as the input and kernel array elements used in its computation:  $(1 \times 1 + 2 \times 2 + 4 \times 3 + 5 \times 4) + (0 \times 0 + 1 \times 1 + 3 \times 2 + 4 \times 3) = 56$ .

<sup>107</sup> <https://discuss.mxnet.io/t/2350>

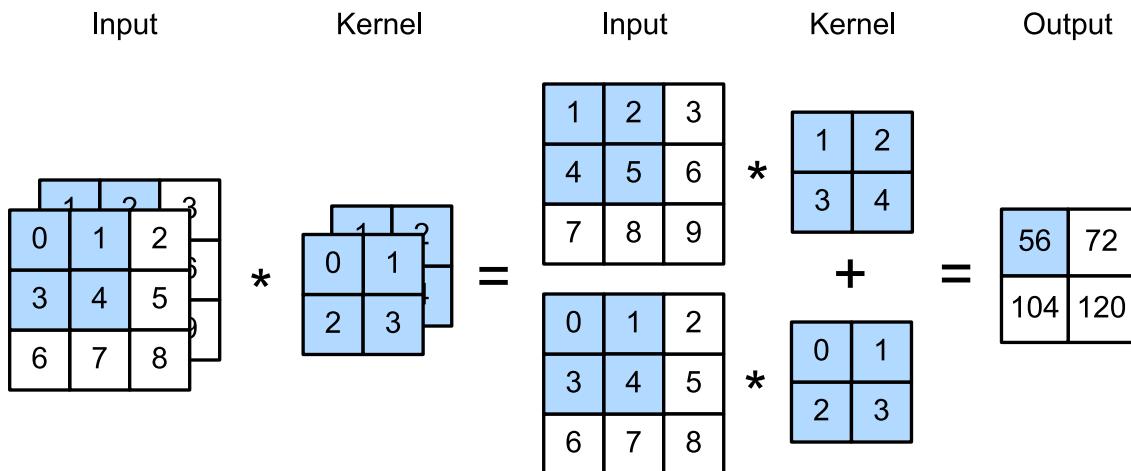


Fig. 8.4.1: Cross-correlation computation with 2 input channels. The shaded portions are the first output element as well as the input and kernel array elements used in its computation:  $(1 \times 1 + 2 \times 2 + 4 \times 3 + 5 \times 4) + (0 \times 0 + 1 \times 1 + 3 \times 2 + 4 \times 3) = 56$ .

To make sure we really understand what's going on here, we can implement cross-correlation operations with multiple input channels ourselves. Notice that all we are doing is performing one cross-correlation operation per channel and then adding up the results using the `add_n` function.

```
import d2l
from mxnet import nd

def corr2d_multi_in(X, K):
    # First, traverse along the 0th dimension (channel dimension) of X and K.
    # Then, add them together by using * to turn the result list into a
    # positional argument of the add_n function
    return nd.add_n(*[d2l.corr2d(x, k) for x, k in zip(X, K)])
```

We can construct the input array `X` and the kernel array `K` corresponding to the values in the above diagram to validate the output of the cross-correlation operation.

```
X = nd.array([[ [0, 1, 2], [3, 4, 5], [6, 7, 8] ],
              [[1, 2, 3], [4, 5, 6], [7, 8, 9]]])
K = nd.array([[ [0, 1], [2, 3] ], [[1, 2], [3, 4]]])

corr2d_multi_in(X, K)
```

```
[[ 56.  72.]
 [104. 120.]]
<NDArray 2x2 @cpu(0)>
```

## 8.4.2 Multiple Output Channels

Regardless of the number of input channels, so far we always ended up with one output channel. However, as we discussed earlier, it turns out to be essential to have multiple channels at each layer. In the most popular neural network architectures, we actually increase the channel dimension as we go higher up in the neural network, typically downsampling to trade off spatial resolution for greater *channel depth*. Intuitively, you

could think of each channel as responding to some different set of features. Reality is a bit more complicated than the most naive interpretations of this intuition since representations aren't learned independent but are rather optimized to be jointly useful. So it may not be that a single channel learns an edge detector but rather that some direction in channel space corresponds to detecting edges.

Denote by  $c_i$  and  $c_o$  the number of input and output channels, respectively, and let  $k_h$  and  $k_w$  be the height and width of the kernel. To get an output with multiple channels, we can create a kernel array of shape  $c_i \times k_h \times k_w$  for each output channel. We concatenate them on the output channel dimension, so that the shape of the convolution kernel is  $c_o \times c_i \times k_h \times k_w$ . In cross-correlation operations, the result on each output channel is calculated from the convolution kernel corresponding to that output channel and takes input from all channels in the input array.

We implement a cross-correlation function to calculate the output of multiple channels as shown below.

```
def corr2d_multi_in_out(X, K):
    # Traverse along the 0th dimension of K, and each time, perform
    # cross-correlation operations with input X. All of the results are merged
    # together using the stack function
    return nd.stack(*[corr2d_multi_in(X, k) for k in K])
```

We construct a convolution kernel with 3 output channels by concatenating the kernel array  $K$  with  $K+1$  (plus one for each element in  $K$ ) and  $K+2$ .

```
K = nd.stack(K, K + 1, K + 2)
K.shape
```

```
(3, 2, 2, 2)
```

Below, we perform cross-correlation operations on the input array  $X$  with the kernel array  $K$ . Now the output contains 3 channels. The result of the first channel is consistent with the result of the previous input array  $X$  and the multi-input channel, single-output channel kernel.

```
corr2d_multi_in_out(X, K)
```

```
[[[ 56.  72.]
 [104. 120.]]

 [[ 76. 100.]
 [148. 172.]]

 [[ 96. 128.]
 [192. 224.]]]
<NDArray 3x2x2 @cpu(0)>
```

### 8.4.3 $1 \times 1$ Convolutional Layer

At first, a  $1 \times 1$  convolution, i.e.  $k_h = k_w = 1$ , doesn't seem to make much sense. After all, a convolution correlates adjacent pixels. A  $1 \times 1$  convolution obviously doesn't. Nonetheless, they are popular operations that are sometimes included in the designs of complex deep networks. Let's see in some detail what it actually does.

Because the minimum window is used, the  $1 \times 1$  convolution loses the ability of larger convolutional layers to recognize patterns consisting of interactions among adjacent elements in the height and width dimensions. The only computation of the  $1 \times 1$  convolution occurs on the channel dimension.

The figure below shows the cross-correlation computation using the  $1 \times 1$  convolution kernel with 3 input channels and 2 output channels. Note that the inputs and outputs have the same height and width. Each element in the output is derived from a linear combination of elements *at the same position* in the input image. You could think of the  $1 \times 1$  convolutional layer as constituting a fully-connected layer applied at every single pixel location to transform the  $c_i$  corresponding input values into  $c_o$  output values. Because this is still a convolutional layer, the weights are tied across pixel location. Thus the  $1 \times 1$  convolutional layer requires  $c_o \times c_i$  weights (plus the bias terms).

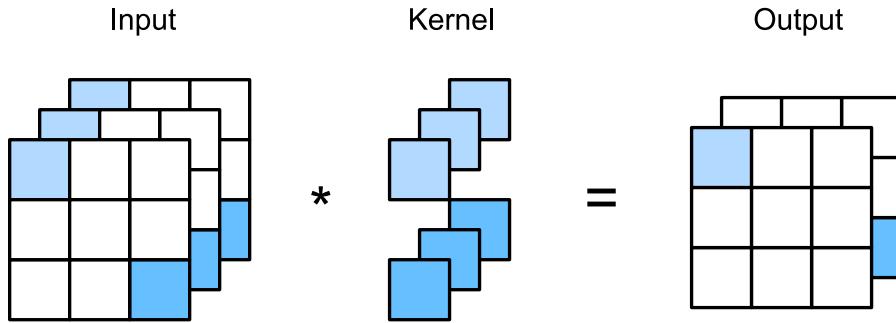


Fig. 8.4.2: The cross-correlation computation uses the  $1 \times 1$  convolution kernel with 3 input channels and 2 output channels. The inputs and outputs have the same height and width.

Let's check whether this works in practice: we implement the  $1 \times 1$  convolution using a fully-connected layer. The only thing is that we need to make some adjustments to the data shape before and after the matrix multiplication.

```
def corr2d_multi_in_out_1x1(X, K):
    c_i, h, w = X.shape
    c_o = K.shape[0]
    X = X.reshape((c_i, h * w))
    K = K.reshape((c_o, c_i))
    Y = nd.dot(K, X) # Matrix multiplication in the fully connected layer
    return Y.reshape((c_o, h, w))
```

When performing  $1 \times 1$  convolution, the above function is equivalent to the previously implemented cross-correlation function `corr2d_multi_in_out`. Let's check this with some reference data.

```
X = nd.random.uniform(shape=(3, 3, 3))
K = nd.random.uniform(shape=(2, 3, 1, 1))

Y1 = corr2d_multi_in_out_1x1(X, K)
Y2 = corr2d_multi_in_out(X, K)

(Y1 - Y2).norm().asscalar() < 1e-6
```

True

#### 8.4.4 Summary

- Multiple channels can be used to extend the model parameters of the convolutional layer.
- The  $1 \times 1$  convolutional layer is equivalent to the fully-connected layer, when applied on a per pixel basis.

- The  $1 \times 1$  convolutional layer is typically used to adjust the number of channels between network layers and to control model complexity.

### 8.4.5 Exercises

1. Assume that we have two convolutional kernels of size  $k_1$  and  $k_2$  respectively (with no nonlinearity in between).
  - Prove that the result of the operation can be expressed by a single convolution.
  - What is the dimensionality of the equivalent single convolution?
  - Is the converse true?
2. Assume an input shape of  $c_i \times h \times w$  and a convolution kernel with the shape  $c_o \times c_i \times k_h \times k_w$ , padding of  $(p_h, p_w)$ , and stride of  $(s_h, s_w)$ .
  - What is the computational cost (multiplications and additions) for the forward computation?
  - What is the memory footprint?
  - What is the memory footprint for the backward computation?
  - What is the computational cost for the backward computation?
3. By what factor does the number of calculations increase if we double the number of input channels  $c_i$  and the number of output channels  $c_o$ ? What happens if we double the padding?
4. If the height and width of the convolution kernel is  $k_h = k_w = 1$ , what is the complexity of the forward computation?
5. Are the variables  $\text{Y1}$  and  $\text{Y2}$  in the last example of this section exactly the same? Why?
6. How would you implement convolutions using matrix multiplication when the convolution window is not  $1 \times 1$ ?

### 8.4.6 Scan the QR Code to Discuss<sup>108</sup>



## 8.5 Pooling

Often, as we process images, we want to gradually reduce the spatial resolution of our hidden representations, aggregating information so that the higher up we go in the network, the larger the receptive field (in the input) to which each hidden node is sensitive.

Often our ultimate task asks some global question about the image, e.g., *does it contain a cat?* So typically the nodes of our final layer should be sensitive to the entire input. By gradually aggregating information, yielding coarser and coarser maps, we accomplish this goal of ultimately learning a global representation, while keeping all of the advantages of convolutional layers at the intermediate layers of processing.

<sup>108</sup> <https://discuss.mxnet.io/t/2351>

Moreover, when detecting lower-level features, such as edges (as discussed in Section 8.2), we often want our representations to be somewhat invariant to translation. For instance, if we take the image  $X$  with a sharp delineation between black and white and shift the whole image by one pixel to the right, i.e.  $Z[i, j] = X[i, j+1]$ , then the output for the new image  $Z$  might be vastly different. The edge will have shifted by one pixel and with it all the activations. In reality, objects hardly ever occur exactly at the same place. In fact, even with a tripod and a stationary object, vibration of the camera due to the movement of the shutter might shift everything by a pixel or so (high-end cameras are loaded with special features to address this problem).

This section introduces pooling layers, which serve the dual purposes of mitigating the sensitivity of convolutional layers to location and of spatially downsampling representations.

### 8.5.1 Maximum Pooling and Average Pooling

Like convolutional layers, pooling operators consist of a fixed-shape window that slides over all regions in the input according to its stride, computing a single output for each location traversed by the fixed-shape window (sometimes known as the *pooling window*). However, unlike the cross-correlation computation of the inputs and kernels in the convolutional layer, the pooling layer contains no parameters (there is no *filter*). Instead, pooling operators are deterministic, typically calculating either the maximum or the average value of the elements in the pooling window. These operations are called *maximum pooling* (*max pooling* for short) and *average pooling*, respectively.

In both cases, as with the cross-correlation operator, we can think of the pooling window as starting from the top left of the input array and sliding across the input array from left to right and top to bottom. At each location that the pooling window hits, it computes the maximum or average value of the input subarray in the window (depending on whether *max* or *average* pooling is employed).

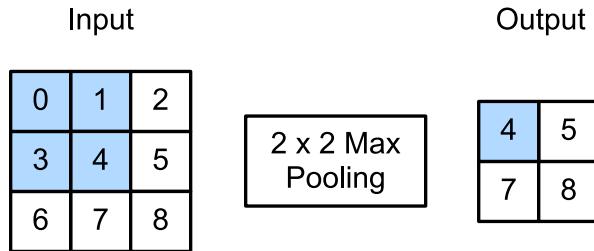


Fig. 8.5.1: Maximum pooling with a pooling window shape of  $2 \times 2$ . The shaded portions represent the first output element and the input element used for its computation:  $\max(0, 1, 3, 4) = 4$

The output array in the figure above has a height of 2 and a width of 2. The four elements are derived from the maximum value of max:

$$\begin{aligned} \max(0, 1, 3, 4) &= 4, \\ \max(1, 2, 4, 5) &= 5, \\ \max(3, 4, 6, 7) &= 7, \\ \max(4, 5, 7, 8) &= 8. \end{aligned} \tag{8.5.1}$$

A pooling layer with a pooling window shape of  $p \times q$  is called a  $p \times q$  pooling layer. The pooling operation is called  $p \times q$  pooling.

Let us return to the object edge detection example mentioned at the beginning of this section. Now we will use the output of the convolutional layer as the input for  $2 \times 2$  maximum pooling. Set the convolutional layer input as  $X$  and the pooling layer output as  $Y$ . Whether or not the values of  $X[i, j]$  and  $X[i, j+1]$  are different, or  $X[i, j+1]$  and  $X[i, j+2]$  are different, the pooling layer outputs all include  $Y[i, j]=1$ .

That is to say, using the  $2 \times 2$  maximum pooling layer, we can still detect if the pattern recognized by the convolutional layer moves no more than one element in height and width.

In the code below, we implement the forward computation of the pooling layer in the `pool2d` function. This function is similar to the `corr2d` function in [Section 8.2](#). However, here we have no kernel, computing the output as either the max or the average of each region in the input..

```
from mxnet import nd
from mxnet.gluon import nn

def pool2d(X, pool_size, mode='max'):
    p_h, p_w = pool_size
    Y = nd.zeros((X.shape[0] - p_h + 1, X.shape[1] - p_w + 1))
    for i in range(Y.shape[0]):
        for j in range(Y.shape[1]):
            if mode == 'max':
                Y[i, j] = X[i:i + p_h, j:j + p_w].max()
            elif mode == 'avg':
                Y[i, j] = X[i:i + p_h, j:j + p_w].mean()
    return Y
```

We can construct the input array `X` in the above diagram to validate the output of the two-dimensional maximum pooling layer.

```
X = nd.array([[0, 1, 2], [3, 4, 5], [6, 7, 8]])
pool2d(X, (2, 2))
```

```
[[4. 5.]
 [7. 8.]]
<NDArray 2x2 @cpu(0)>
```

At the same time, we experiment with the average pooling layer.

```
pool2d(X, (2, 2), 'avg')
```

```
[[2. 3.]
 [5. 6.]]
<NDArray 2x2 @cpu(0)>
```

## 8.5.2 Padding and Stride

As with convolutional layers, pooling layers can also change the output shape. And as before, we can alter the operation to achieve a desired output shape by padding the input and adjusting the stride. We can demonstrate the use of padding and strides in pooling layers via the two-dimensional maximum pooling layer `MaxPool2D` shipped in MXNet Gluon's `nn` module. We first construct an input data of shape  $(1, 1, 4, 4)$ , where the first two dimensions are batch and channel.

```
X = nd.arange(16).reshape((1, 1, 4, 4))
X
```

```
[[[[ 0. 1. 2. 3.]
   [ 4. 5. 6. 7.]
```

(continues on next page)

(continued from previous page)

```
[ 8.  9. 10. 11.]  
[12. 13. 14. 15.]]]  
<NDArray 1x1x4x4 @cpu(0)>
```

By default, the stride in the `MaxPool2D` class has the same shape as the pooling window. Below, we use a pooling window of shape  $(3, 3)$ , so we get a stride shape of  $(3, 3)$  by default.

```
pool2d = nn.MaxPool2D(3)  
# Because there are no model parameters in the pooling layer, we do not need  
# to call the parameter initialization function  
pool2d(X)
```

```
[[[[10.]]]  
<NDArray 1x1x1x1 @cpu(0)>
```

The stride and padding can be manually specified.

```
pool2d = nn.MaxPool2D(3, padding=1, strides=2)  
pool2d(X)
```

```
[[[[ 5.  7.]  
[13. 15.]]]  
<NDArray 1x1x2x2 @cpu(0)>
```

Of course, we can specify an arbitrary rectangular pooling window and specify the padding and stride for height and width, respectively.

```
pool2d = nn.MaxPool2D((2, 3), padding=(1, 2), strides=(2, 3))  
pool2d(X)
```

```
[[[[ 0.  3.]  
[ 8. 11.]  
[12. 15.]]]  
<NDArray 1x1x3x2 @cpu(0)>
```

### 8.5.3 Multiple Channels

When processing multi-channel input data, the pooling layer pools each input channel separately, rather than adding the inputs of each channel by channel as in a convolutional layer. This means that the number of output channels for the pooling layer is the same as the number of input channels. Below, we will concatenate arrays `X` and `X+1` on the channel dimension to construct an input with 2 channels.

```
X = nd.concat(X, X + 1, dim=1)  
X
```

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

(continues on next page)

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```
[[ 1.  2.  3.  4.]
 [ 5.  6.  7.  8.]
 [ 9. 10. 11. 12.]
 [13. 14. 15. 16.]])
<NDArray 1x2x4x4 @cpu(0)>
```

As we can see, the number of output channels is still 2 after pooling.

```
pool2d = nn.MaxPool2D(3, padding=1, strides=2)
pool2d(X)
```

```
[[[[ 5.  7.]
   [13. 15.]]
 [[ 6.  8.]
   [14. 16.]])
<NDArray 1x2x2x2 @cpu(0)>
```

#### 8.5.4 Summary

- Taking the input elements in the pooling window, the maximum pooling operation assigns the maximum value as the output and the average pooling operation assigns the average value as the output.
- One of the major functions of a pooling layer is to alleviate the excessive sensitivity of the convolutional layer to location.
- We can specify the padding and stride for the pooling layer.
- Maximum pooling, combined with a stride larger than 1 can be used to reduce the resolution.
- The pooling layer's number of output channels is the same as the number of input channels.

#### 8.5.5 Exercises

1. Can you implement average pooling as a special case of a convolution layer? If so, do it.
2. Can you implement max pooling as a special case of a convolution layer? If so, do it.
3. What is the computational cost of the pooling layer? Assume that the input to the pooling layer is of size  $c \times h \times w$ , the pooling window has a shape of  $p_h \times p_w$  with a padding of  $(p_h, p_w)$  and a stride of  $(s_h, s_w)$ .
4. Why do you expect maximum pooling and average pooling to work differently?
5. Do we need a separate minimum pooling layer? Can you replace it with another operation?
6. Is there another operation between average and maximum pooling that you could consider (hint - recall the softmax)? Why might it not be so popular?

#### 8.5.6 Scan the QR Code to Discuss<sup>109</sup>

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<sup>109</sup> <https://discuss.mxnet.io/t/2352>



## 8.6 Convolutional Neural Networks (LeNet)

We are now ready to put all of the tools together to deploy your first fully-functional convolutional neural network. In our first encounter with image data we applied a multilayer perceptron (Section 6.2) to pictures of clothing in the Fashion-MNIST data set. Each image in Fashion-MNIST consisted of a two-dimensional  $28 \times 28$  matrix. To make this data amenable to multilayer perceptrons which anticipate receiving inputs as one-dimensional fixed-length vectors, we first flattened each image, yielding vectors of length 784, before processing them with a series of fully-connected layers.

Now that we have introduced convolutional layers, we can keep the image in its original spatially-organized grid, processing it with a series of successive convolutional layers. Moreover, because we are using convolutional layers, we can enjoy a considerable savings in the number of parameters required.

In this section, we will introduce one of the first published convolutional neural networks whose benefit was first demonstrated by Yann LeCun, then a researcher at AT&T Bell Labs, for the purpose of recognizing handwritten digits in images—LeNet5<sup>110</sup>. In the 90s, their experiments with LeNet gave the first compelling evidence that it was possible to train convolutional neural networks by backpropagation. Their model achieved outstanding results at the time (only matched by Support Vector Machines at the time) and was adopted to recognize digits for processing deposits in ATM machines. Some ATMs still run the code that Yann and his colleague Leon Bottou wrote in the 1990s!

### 8.6.1 LeNet

In a rough sense, we can think LeNet as consisting of two parts: (i) a block of convolutional layers; and (ii) a block of fully-connected layers. Before getting into the weeds, let's briefly review the model in Fig. 8.6.1.

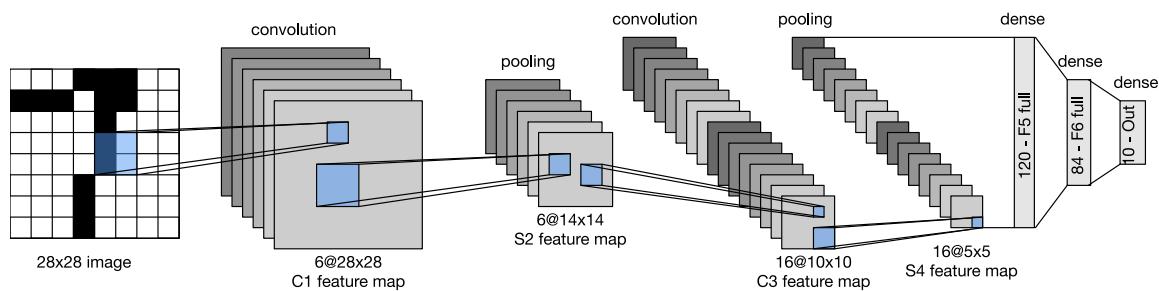


Fig. 8.6.1: Data flow in LeNet 5. The input is a handwritten digit, the output a probability over 10 possible outcomes.

<sup>110</sup> <http://yann.lecun.com/exdb/lenet/>

The basic units in the convolutional block are a convolutional layer and a subsequent average pooling layer (note that max-pooling works better, but it had not been invented in the 90s yet). The convolutional layer is used to recognize the spatial patterns in the image, such as lines and the parts of objects, and the subsequent average pooling layer is used to reduce the dimensionality. The convolutional layer block is composed of repeated stacks of these two basic units. Each convolutional layer uses a  $5 \times 5$  kernel and processes each output with a sigmoid activation function (again, note that ReLUs are now known to work more reliably, but had not been invented yet). The first convolutional layer has 6 output channels, and second convolutional layer increases channel depth further to 16.

However, coinciding with this increase in the number of channels, the height and width are shrunk considerably. Therefore, increasing the number of output channels makes the parameter sizes of the two convolutional layers similar. The two average pooling layers are of size  $2 \times 2$  and take stride 2 (note that this means they are non-overlapping). In other words, the pooling layer downsamples the representation to be precisely *one quarter* the pre-pooling size.

The convolutional block emits an output with size given by (batch size, channel, height, width). Before we can pass the convolutional block's output to the fully-connected block, we must flatten each example in the mini-batch. In other words, we take this 4D input and transform it into the 2D input expected by fully-connected layers: as a reminder, the first dimension indexes the examples in the mini-batch and the second gives the flat vector representation of each example. LeNet's fully-connected layer block has three fully-connected layers, with 120, 84, and 10 outputs, respectively. Because we are still performing classification, the 10 dimensional output layer corresponds to the number of possible output classes.

While getting to the point where you truly understand what's going on inside LeNet may have taken a bit of work, you can see below that implementing it in a modern deep learning library is remarkably simple. Again, we'll rely on the Sequential class.

```
import d2l
from mxnet import autograd, gluon, init, nd
from mxnet.gluon import nn

net = nn.Sequential()
net.add(nn.Conv2D(channels=6, kernel_size=5, padding=2, activation='sigmoid'),
       nn.AvgPool2D(pool_size=2, strides=2),
       nn.Conv2D(channels=16, kernel_size=5, activation='sigmoid'),
       nn.AvgPool2D(pool_size=2, strides=2),
       # Dense will transform the input of the shape (batch size, channel,
       # height, width) into the input of the shape (batch size,
       # channel * height * width) automatically by default
       nn.Dense(120, activation='sigmoid'),
       nn.Dense(84, activation='sigmoid'),
       nn.Dense(10))
```

As compared to the original network, we took the liberty of replacing the Gaussian activation in the last layer by a regular dense layer, which tends to be significantly more convenient to train. Other than that, this network matches the historical definition of LeNet5. Next, we feed a single-channel example of size  $28 \times 28$  into the network and perform a forward computation layer by layer printing the output shape at each layer to make sure we understand what's happening here.

```
X = nd.random.uniform(shape=(1, 1, 28, 28))
net.initialize()
for layer in net:
    X = layer(X)
    print(layer.name, 'output shape:\t', X.shape)
```

```
conv0 output shape: (1, 6, 28, 28)
pool0 output shape: (1, 6, 14, 14)
conv1 output shape: (1, 16, 10, 10)
pool1 output shape: (1, 16, 5, 5)
dense0 output shape: (1, 120)
dense1 output shape: (1, 84)
dense2 output shape: (1, 10)
```

Note that the height and width of the representation at each layer throughout the convolutional block is reduced (compared to the previous layer). The convolutional layer uses a kernel with a height and width of 5, which with only 2 pixels of padding in the first convolutional layer and none in the second convolutional layer leads to reductions in both height and width by 0 and 4 pixels, respectively. Moreover each pooling layer halves the height and width. However, as we go up the stack of layers, the number of channels increases layer-over-layer from 1 in the input to 6 after the first convolutional layer and 16 after the second layer. Then, the fully-connected layer reduces dimensionality layer by layer, until emitting an output that matches the number of image classes.

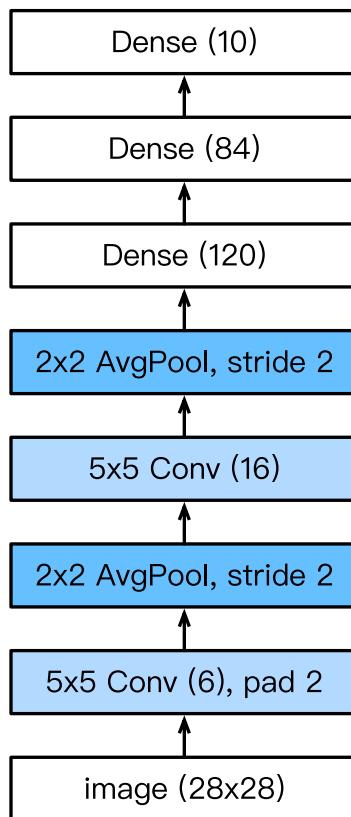


Fig. 8.6.2: Compressed notation for LeNet5

### 8.6.2 Data Acquisition and Training

Now that we've implemented the model, we might as well run some experiments to see what we can accomplish with the LeNet model. While it might serve nostalgia to train LeNet on the original MNIST dataset, that dataset has become too easy, with MLPs getting over 98% accuracy, so it would be hard to see the benefits of convolutional networks. Thus we will stick with Fashion-MNIST as our dataset because while it has the same shape ( $28 \times 28$  images), this dataset is notably more challenging.

```
batch_size = 256
train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size=batch_size)
```

While convolutional networks may have few parameters, they can still be significantly more expensive to compute than a similarly deep multilayer perceptron so if you have access to a GPU, this might be a good time to put it into action to speed up training.

For evaluation, we need to make a slight modification to the `evaluate_accuracy` function that we described in Section 5.6. Since the full dataset lives on the CPU, we need to copy it to the GPU before we can compute our models. This is accomplished via the `as_in_context` function described in Section 7.6.

```
# Save to the d2l package
def evaluate_accuracy_gpu(net, data_iter, ctx=None):
    if not ctx: # Query the first device the first parameter is on.
        ctx = list(net.collect_params().values())[0].list_ctx()[0]
    metric = d2l.Accumulator(2) # num_corrected_examples, num_examples
    for X, y in data_iter:
        X, y = X.as_in_context(ctx), y.as_in_context(ctx)
        metric.add(d2l.accuracy(net(X), y), y.size)
    return metric[0]/metric[1]
```

We also need to update our training function to deal with GPUs. Unlike the `train_epoch_ch3` defined in Section 5.6, we now need to move each batch of data to our designated context (hopefully, the GPU) prior to making the forward and backward passes.

The training function `train_ch5` is also very similar to `train_ch3` defined in Section 5.6. Since we will deal with networks with tens of layers now, the function will only support Gluon models. We initialize the model parameters on the device indicated by `ctx`, this time using the Xavier initializer. The loss function and the training algorithm still use the cross-entropy loss function and mini-batch stochastic gradient descent. Since each epoch takes tens of second to run, we visualize the training loss in a finer granularity.

```
# Save to the d2l package.
def train_ch5(net, train_iter, test_iter, num_epochs, lr, ctx=d2l.try_gpu()):
    net.initialize(force_reinit=True, ctx=ctx, init=init.Xavier())
    loss = gluon.loss.SoftmaxCrossEntropyLoss()
    trainer = gluon.Trainer(net.collect_params(),
                           'sgd', {'learning_rate': lr})
    animator = d2l.Animator(xlabel='epoch', xlim=[0,num_epochs],
                           legend=['train loss','train acc','test acc'])
    timer = d2l.Timer()
    for epoch in range(num_epochs):
        metric = d2l.Accumulator(3) # train_loss, train_acc, num_examples
        for i, (X, y) in enumerate(train_iter):
            timer.start()
            # Here is the only difference compared to train_epoch_ch3
            X, y = X.as_in_context(ctx), y.as_in_context(ctx)
            with autograd.record():
                y_hat = net(X)
                l = loss(y_hat, y)
            l.backward()
            trainer.step(X.shape[0])
            metric.add(l.sum().asscalar(), d2l.accuracy(y_hat, y), X.shape[0])
            timer.stop()
        train_loss, train_acc = metric[0]/metric[2], metric[1]/metric[2]
        animator.add(epoch + 1, (train_loss, train_acc))
    test_acc = eval_accuracy(net, test_iter, ctx)
    print('test accuracy: %f' % test_acc)
```

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```

if (i+1) % 50 == 0:
    animator.add(epoch + i/len(train_iter),
                 (train_loss, train_acc, None))
    test_acc = evaluate_accuracy_gpu(net, test_iter)
    animator.add(epoch+1, (None, None, test_acc))
print('loss %.3f, train acc %.3f, test acc %.3f' % (
    train_loss, train_acc, test_acc))
print('%.1f examples/sec on %s' % (metric[2]*num_epochs/timer.sum(), ctx))

```

Now let's train the model.

```

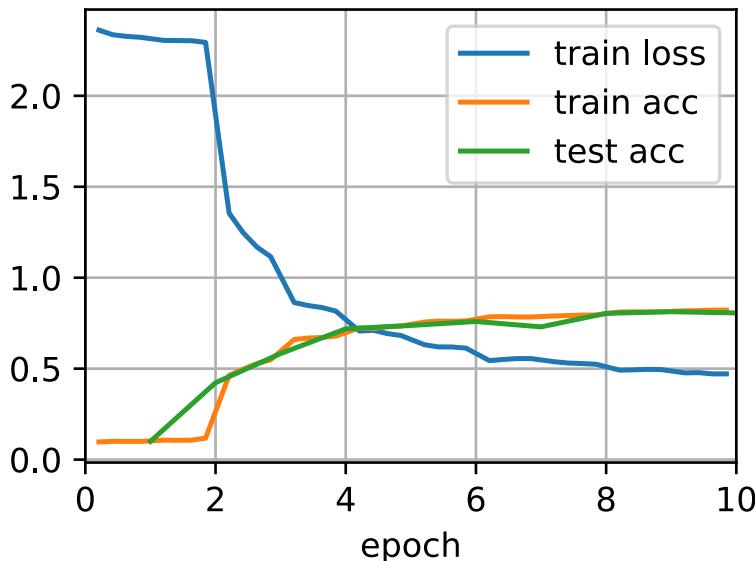
lr, num_epochs = 0.9, 10
train_ch5(net, train_iter, test_iter, num_epochs, lr)

```

```

loss 0.471, train acc 0.822, test acc 0.806
60721.4 examples/sec on gpu(0)

```



### 8.6.3 Summary

- A convolutional neural network (in short, ConvNet) is a network using convolutional layers.
- In a ConvNet we alternate between convolutions, nonlinearities and often also pooling operations.
- Ultimately the resolution is reduced prior to emitting an output via one (or more) dense layers.
- LeNet was the first successful deployment of such a network.

### 8.6.4 Exercises

1. Replace the average pooling with max pooling. What happens?
2. Try to construct a more complex network based on LeNet to improve its accuracy.

- Adjust the convolution window size.
  - Adjust the number of output channels.
  - Adjust the activation function (ReLU?).
  - Adjust the number of convolution layers.
  - Adjust the number of fully connected layers.
  - Adjust the learning rates and other training details (initialization, epochs, etc.)
3. Try out the improved network on the original MNIST dataset.
  4. Display the activations of the first and second layer of LeNet for different inputs (e.g. sweaters, coats).

#### 8.6.5 Scan the QR Code to Discuss<sup>111</sup>



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<sup>111</sup> <https://discuss.mxnet.io/t/2353>



## MODERN CONVOLUTIONAL NETWORKS

Now that we understand the basics of wiring together convolutional neural networks, we will take you through a tour of modern deep learning. In this chapter, each section will correspond to a significant neural network architecture that was at some point (or currently) the base model upon which an enormous amount of research and projects were built. Each of these networks was at briefly a dominant architecture and many were at one point winners or runners-up in the famous ImageNet competition, which has served as a barometer of progress on supervised learning in computer vision since 2010.

These models include AlexNet, the first large-scale network deployed to beat conventional computer vision methods on a large-scale vision challenge; the VGG network, which makes use of a number of repeating blocks of elements; the network in network (NiN) which convolves whole neural networks patch-wise over inputs; the GoogLeNet, which makes use of networks with parallel concatenations (GoogLeNet); residual networks (ResNet) which are currently the most popular go-to architecture today, and densely connected networks (DenseNet), which are expensive to compute but have set some recent benchmarks.

### 9.1 Deep Convolutional Neural Networks (AlexNet)

Although convolutional neural networks were well known in the computer vision and machine learning communities following the introduction of LeNet, they did not immediately dominate the field. Although LeNet achieved good results on early small data sets, the performance and feasibility of training convolutional networks on larger, more realistic datasets had yet to be established. In fact, for much of the intervening time between the early 1990s and the watershed results of 2012, neural networks were often surpassed by other machine learning methods, such as support vector machines.

For computer vision, this comparison is perhaps not fair. That's although the inputs to convolutional networks consist of raw or lightly-processed (e.g., by centering) pixel values, practitioners would never feed raw pixels into traditional models. Instead, typical computer vision pipelines consisted of manually engineering feature extraction pipelines. Rather than *learn the features*, the features were *crafted*. Most of the progress came from having more clever ideas for features, and the learning algorithm was often relegated to an afterthought.

Although some neural network accelerators were available in the 1990s, they were not yet sufficiently powerful to make deep multichannel, multilayer convolutional neural networks with a large number of parameters. Moreover, datasets were still relatively small. Added to these obstacles, key tricks for training neural networks including parameter initialization heuristics, clever variants of stochastic gradient descent, non-squashing activation functions, and effective regularization techniques were still missing.

Thus, rather than training *end-to-end* (pixel to classification) systems, classical pipelines looked more like this:

1. Obtain an interesting dataset. In early days, these datasets required expensive sensors (at the time, 1 megapixel images were state of the art).

2. Preprocess the dataset with hand-crafted features based on some knowledge of optics, geometry, other analytic tools, and occasionally on the serendipitous discoveries of lucky graduate students.
3. Feed the data through a standard set of feature extractors such as SIFT<sup>112</sup>, the Scale-Invariant Feature Transform, or SURF<sup>113</sup>, the Speeded-Up Robust Features, or any number of other hand-tuned pipelines.
4. Dump the resulting representations into your favorite classifier, likely a linear model or kernel method, to learn a classifier.

If you spoke to machine learning researchers, they believed that machine learning was both important and beautiful. Elegant theories proved the properties of various classifiers. The field of machine learning was thriving, rigorous and eminently useful. However, if you spoke to a computer vision researcher, you'd hear a very different story. The dirty truth of image recognition, they'd tell you, is that features, not learning algorithms, drove progress. Computer vision researchers justifiably believed that a slightly bigger or cleaner dataset or a slightly improved feature-extraction pipeline mattered far more to the final accuracy than any learning algorithm.

### 9.1.1 Learning Feature Representation

Another way to cast the state of affairs is that the most important part of the pipeline was the representation. And up until 2012 the representation was calculated mechanically. In fact, engineering a new set of feature functions, improving results, and writing up the method was a prominent genre of paper. SIFT<sup>114</sup>, SURF<sup>115</sup>, HOG<sup>116</sup>, Bags of visual words<sup>117</sup> and similar feature extractors ruled the roost.

Another group of researchers, including Yann LeCun, Geoff Hinton, Yoshua Bengio, Andrew Ng, Shun-ichi Amari, and Juergen Schmidhuber, had different plans. They believed that features themselves ought to be learned. Moreover, they believed that to be reasonably complex, the features ought to be hierarchically composed with multiple jointly learned layers, each with learnable parameters. In the case of an image, the lowest layers might come to detect edges, colors, and textures. Indeed, [33] proposed a new variant of a convolutional neural network which achieved excellent performance in the ImageNet challenge.

Interestingly in the lowest layers of the network, the model learned feature extractors that resembled some traditional filters. The figure below is reproduced from this paper and describes lower-level image descriptors.

Higher layers in the network might build upon these representations to represent larger structures, like eyes, noses, blades of grass, etc. Even higher layers might represent whole objects like people, airplanes, dogs, or frisbees. Ultimately, the final hidden state learns a compact representation of the image that summarizes its contents such that data belonging to different categories be separated easily.

While the ultimate breakthrough for many-layered convolutional networks came in 2012, a core group of researchers had dedicated themselves to this idea, attempting to learn hierarchical representations of visual data for many years. The ultimate breakthrough in 2012 can be attributed to two key factors.

### Missing Ingredient - Data

Deep models with many layers require large amounts of data in order to enter the regime where they significantly outperform traditional methods based on convex optimizations (e.g. linear and kernel methods). However, given the limited storage capacity of computers, the relative expense of sensors, and the comparatively tighter research budgets in the 1990s, most research relied on tiny datasets. Numerous papers

<sup>112</sup> [https://en.wikipedia.org/wiki/Scale-invariant\\_feature\\_transform](https://en.wikipedia.org/wiki/Scale-invariant_feature_transform)

<sup>113</sup> [https://en.wikipedia.org/wiki/Speeded\\_up\\_robust\\_features](https://en.wikipedia.org/wiki/Speeded_up_robust_features)

<sup>114</sup> [https://en.wikipedia.org/wiki/Scale-invariant\\_feature\\_transform](https://en.wikipedia.org/wiki/Scale-invariant_feature_transform)

<sup>115</sup> [https://en.wikipedia.org/wiki/Speeded\\_up\\_robust\\_features](https://en.wikipedia.org/wiki/Speeded_up_robust_features)

<sup>116</sup> [https://en.wikipedia.org/wiki/Histogram\\_of\\_oriented\\_gradients](https://en.wikipedia.org/wiki/Histogram_of_oriented_gradients)

<sup>117</sup> [https://en.wikipedia.org/wiki/Bag-of-words\\_model\\_in\\_computer\\_vision](https://en.wikipedia.org/wiki/Bag-of-words_model_in_computer_vision)

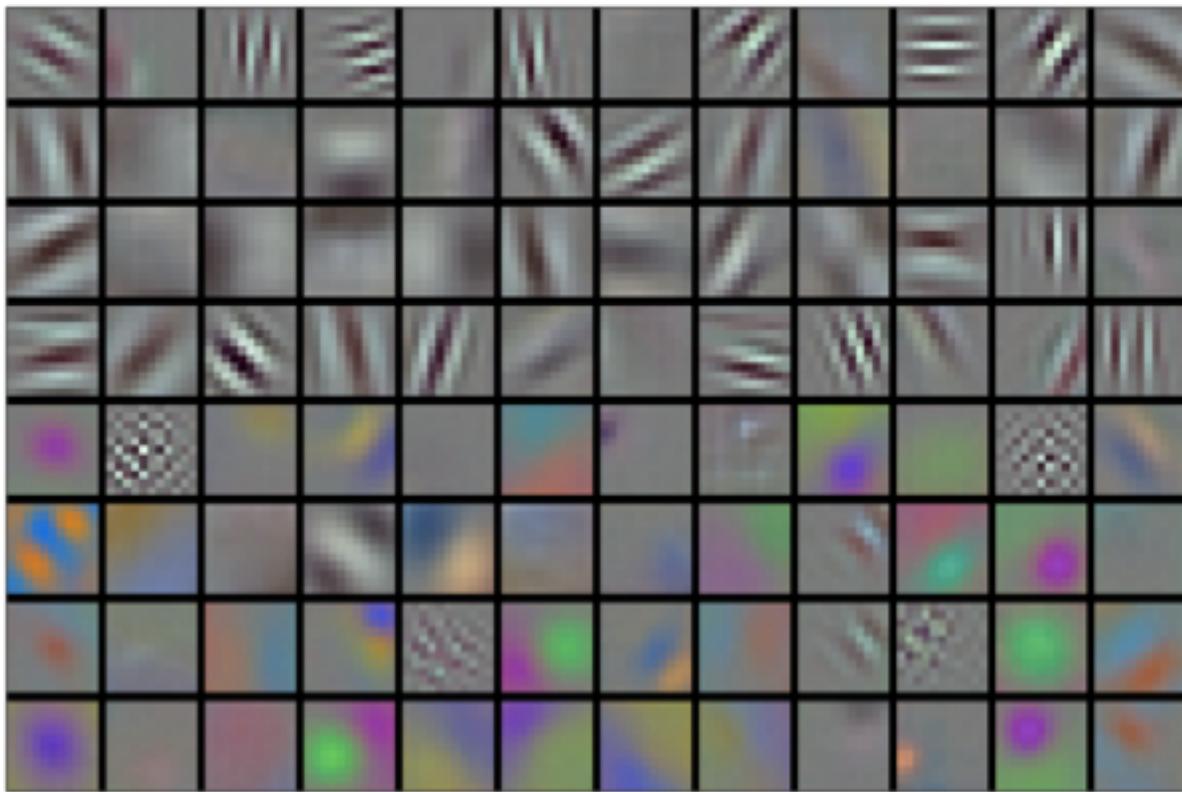


Fig. 9.1.1: Image filters learned by the first layer of AlexNet

addressed the UCI collection of datasets, many of which contained only hundreds or (a few) thousands of images captured in unnatural settings with low resolution.

In 2009, the ImageNet data set was released, challenging researchers to learn models from 1 million examples, 1,000 each from 1,000 distinct categories of objects. The researchers, led by Fei-Fei Li, who introduced this dataset leveraged Google Image Search to prefilter large candidate sets for each category and employed the Amazon Mechanical Turk crowdsourcing pipeline to confirm for each image whether it belonged to the associated category. This scale was unprecedented. The associated competition, dubbed the ImageNet Challenge pushed computer vision and machine learning research forward, challenging researchers to identify which models performed best at a greater scale than academics had previously considered.

### **Missing Ingredient - Hardware**

Deep learning models are voracious consumers of compute cycles. Training can take hundreds of epochs, and each iteration requires passing data through many layers of computationally-expensive linear algebra operations. This is one of the main reasons why in the 90s and early 2000s, simple algorithms based on the more-efficiently optimized convex objectives were preferred.

Graphical processing units (GPUs) proved to be a game changer in make deep learning feasible. These chips had long been developed for accelerating graphics processing to benefit computer games. In particular, they were optimized for high throughput 4x4 matrix-vector products, which are needed for many computer graphics tasks. Fortunately, this math is strikingly similar to that required to calculate convolutional layers. Around that time, NVIDIA and ATI had begun optimizing GPUs for general compute operations, going as far as to market them as General Purpose GPUs (GPGPU).

To provide some intuition, consider the cores of a modern microprocessor (CPU). Each of the cores is fairly

powerful running at a high clock frequency and sporting large caches (up to several MB of L3). Each core is well-suited to executing a wide range of instructions, with branch predictors, a deep pipeline, and other bells and whistles that enable it to run a large variety of programs. This apparent strength, however, is also its Achilles heel: general purpose cores are very expensive to build. They require lots of chip area, a sophisticated support structure (memory interfaces, caching logic between cores, high speed interconnects, etc.), and they're comparatively bad at any single task. Modern laptops have up to 4 cores, and even high end servers rarely exceed 64 cores, simply because it is not cost effective.

By comparison, GPUs consist of 100-1000 small processing elements (the details differ somewhat between NVIDIA, ATI, ARM and other chip vendors), often grouped into larger groups (NVIDIA calls them warps). While each core is relatively weak, sometimes even running at sub-1GHz clock frequency, it is the total number of such cores that makes GPUs orders of magnitude faster than CPUs. For instance, NVIDIA's latest Volta generation offers up to 120 TFlops per chip for specialized instructions (and up to 24 TFlops for more general purpose ones), while floating point performance of CPUs has not exceeded 1 TFlop to date. The reason for why this is possible is actually quite simple: firstly, power consumption tends to grow *quadratically* with clock frequency. Hence, for the power budget of a CPU core that runs 4x faster (a typical number), you can use 16 GPU cores at 1/4 the speed, which yields  $16 \times 1/4 = 4$ x the performance. Furthermore, GPU cores are much simpler (in fact, for a long time they weren't even *able* to execute general purpose code), which makes them more energy efficient. Lastly, many operations in deep learning require high memory bandwidth. Again, GPUs shine here with buses that are at least 10x as wide as many CPUs.

Back to 2012. A major breakthrough came when Alex Krizhevsky and Ilya Sutskever implemented a deep convolutional neural network that could run on GPU hardware. They realized that the computational bottlenecks in CNNs (convolutions and matrix multiplications) are all operations that could be parallelized in hardware. Using two NVIDIA GTX 580s with 3GB of memory, they implemented fast convolutions. The code `cuda-convnet`<sup>118</sup> was good enough that for several years it was the industry standard and powered the first couple years of the deep learning boom.

### 9.1.2 AlexNet

AlexNet was introduced in 2012, named after Alex Krizhevsky, the first author of the breakthrough ImageNet classification paper [33]. AlexNet, which employed an 8-layer convolutional neural network, won the ImageNet Large Scale Visual Recognition Challenge 2012 by a phenomenally large margin. This network proved, for the first time, that the features obtained by learning can transcend manually-designed features, breaking the previous paradigm in computer vision. The architectures of AlexNet and LeNet are *very similar*, as the diagram below illustrates. Note that we provide a slightly streamlined version of AlexNet removing some of the design quirks that were needed in 2012 to make the model fit on two small GPUs.

The design philosophies of AlexNet and LeNet are very similar, but there are also significant differences. First, AlexNet is much deeper than the comparatively small LeNet5. AlexNet consists of eight layers: five convolutional layers, two fully-connected hidden layers, and one fully-connected output layer. Second, AlexNet used the ReLU instead of the sigmoid as its activation function. Let's delve into the details below.

#### Architecture

In AlexNet's first layer, the convolution window shape is  $11 \times 11$ . Since most images in ImageNet are more than ten times higher and wider than the MNIST images, objects in ImageNet data tend to occupy more pixels. Consequently, a larger convolution window is needed to capture the object. The convolution window shape in the second layer is reduced to  $5 \times 5$ , followed by  $3 \times 3$ . In addition, after the first, second, and fifth convolutional layers, the network adds maximum pooling layers with a window shape of  $3 \times 3$  and a stride of 2. Moreover, AlexNet has ten times more convolution channels than LeNet.

---

<sup>118</sup> <https://code.google.com/archive/p/cuda-convnet/>

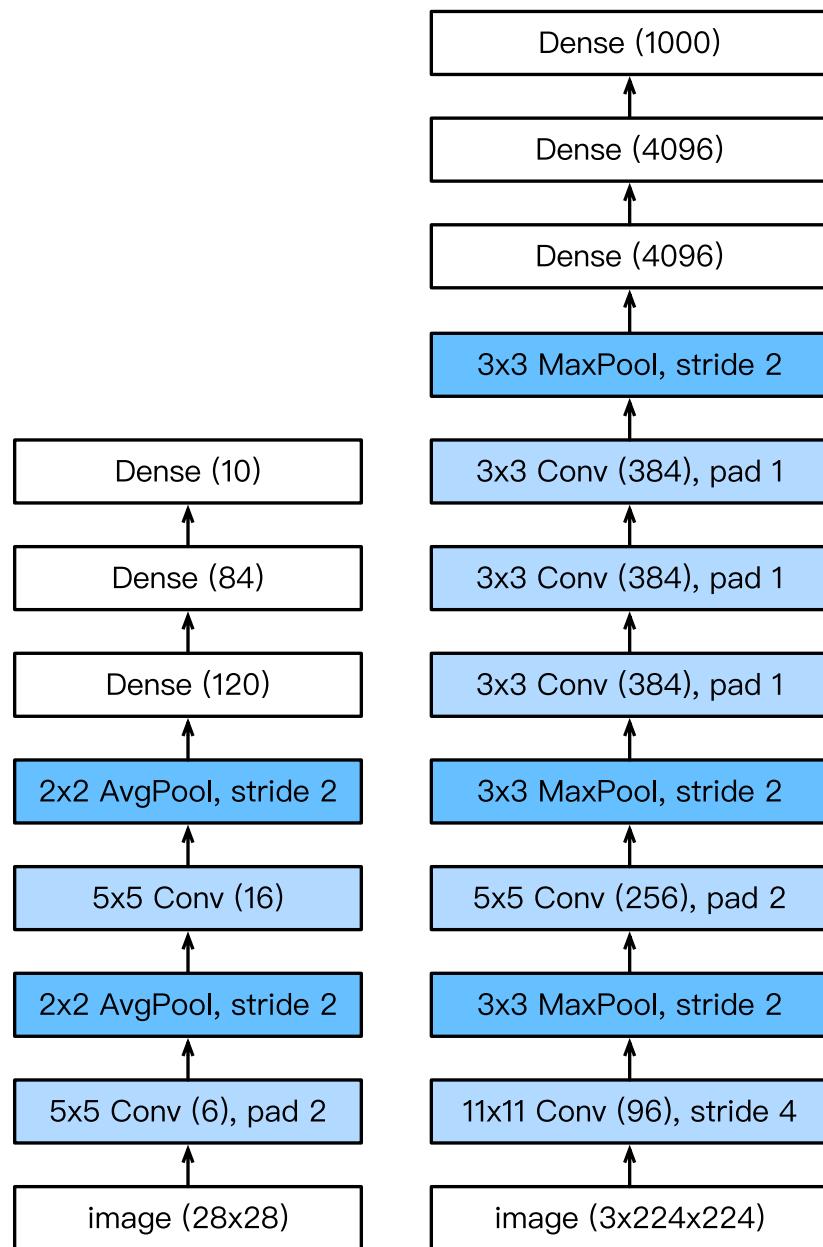


Fig. 9.1.2: LeNet (left) and AlexNet (right)

After the last convolutional layer are two fully-connected layers with 4096 outputs. These two huge fully-connected layers produce model parameters of nearly 1 GB. Due to the limited memory in early GPUs, the original AlexNet used a dual data stream design, so that each of their two GPUs could be responsible for storing and computing only its half of the model. Fortunately, GPU memory is comparatively abundant now, so we rarely need to break up models across GPUs these days (our version of the AlexNet model deviates from the original paper in this aspect).

## Activation Functions

Second, AlexNet changed the sigmoid activation function to a simpler ReLU activation function. On the one hand, the computation of the ReLU activation function is simpler. For example, it does not have the exponentiation operation found in the sigmoid activation function. On the other hand, the ReLU activation function makes model training easier when using different parameter initialization methods. This is because, when the output of the sigmoid activation function is very close to 0 or 1, the gradient of these regions is almost 0, so that back propagation cannot continue to update some of the model parameters. In contrast, the gradient of the ReLU activation function in the positive interval is always 1. Therefore, if the model parameters are not properly initialized, the sigmoid function may obtain a gradient of almost 0 in the positive interval, so that the model cannot be effectively trained.

## Capacity Control and Preprocessing

AlexNet controls the model complexity of the fully-connected layer by dropout (Section 6.6), while LeNet only uses weight decay. To augment the data even further, the training loop of AlexNet added a great deal of image augmentation, such as flipping, clipping, and color changes. This makes the model more robust and the larger sample size effectively reduces overfitting. We will discuss data augmentation in greater detail in Section 14.1.

```
import d2l
from mxnet import gluon, nd
from mxnet.gluon import nn

net = nn.Sequential()
# Here, we use a larger 11 x 11 window to capture objects. At the same time,
# we use a stride of 4 to greatly reduce the height and width of the output.
# Here, the number of output channels is much larger than that in LeNet
net.add(nn.Conv2D(96, kernel_size=11, strides=4, activation='relu'),
        nn.MaxPool2D(pool_size=3, strides=2),
        # Make the convolution window smaller, set padding to 2 for consistent
        # height and width across the input and output, and increase the
        # number of output channels
        nn.Conv2D(256, kernel_size=5, padding=2, activation='relu'),
        nn.MaxPool2D(pool_size=3, strides=2),
        # Use three successive convolutional layers and a smaller convolution
        # window. Except for the final convolutional layer, the number of
        # output channels is further increased. Pooling layers are not used to
        # reduce the height and width of input after the first two
        # convolutional layers
        nn.Conv2D(384, kernel_size=3, padding=1, activation='relu'),
        nn.Conv2D(384, kernel_size=3, padding=1, activation='relu'),
        nn.Conv2D(256, kernel_size=3, padding=1, activation='relu'),
        nn.MaxPool2D(pool_size=3, strides=2),
        # Here, the number of outputs of the fully connected layer is several
```

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```
# times larger than that in LeNet. Use the dropout layer to mitigate
# overfitting
nn.Dense(4096, activation="relu"), nn.Dropout(0.5),
nn.Dense(4096, activation="relu"), nn.Dropout(0.5),
# Output layer. Since we are using Fashion-MNIST, the number of
# classes is 10, instead of 1000 as in the paper
nn.Dense(10))
```

We construct a single-channel data instance with both height and width of 224 to observe the output shape of each layer. It matches our diagram above.

```
X = nd.random.uniform(shape=(1, 1, 224, 224))
net.initialize()
for layer in net:
    X = layer(X)
    print(layer.name, 'output shape:\t', X.shape)
```

```
conv0 output shape: (1, 96, 54, 54)
pool0 output shape: (1, 96, 26, 26)
conv1 output shape: (1, 256, 26, 26)
pool1 output shape: (1, 256, 12, 12)
conv2 output shape: (1, 384, 12, 12)
conv3 output shape: (1, 384, 12, 12)
conv4 output shape: (1, 256, 12, 12)
pool2 output shape: (1, 256, 5, 5)
dense0 output shape: (1, 4096)
dropout0 output shape: (1, 4096)
dense1 output shape: (1, 4096)
dropout1 output shape: (1, 4096)
dense2 output shape: (1, 10)
```

### 9.1.3 Reading Data

Although AlexNet uses ImageNet in the paper, we use Fashion-MNIST here since training an ImageNet model to convergence could take hours or days even on a modern GPU. One of the problems with applying AlexNet directly on Fashion-MNIST is that our images are lower resolution ( $28 \times 28$  pixels) than ImageNet images. To make things work, we upsample them to  $244 \times 244$  (generally not a smart practice, but we do it here to be faithful to the AlexNet architecture). We perform this resizing with the `resize` argument in `load_data_fashion_mnist`.

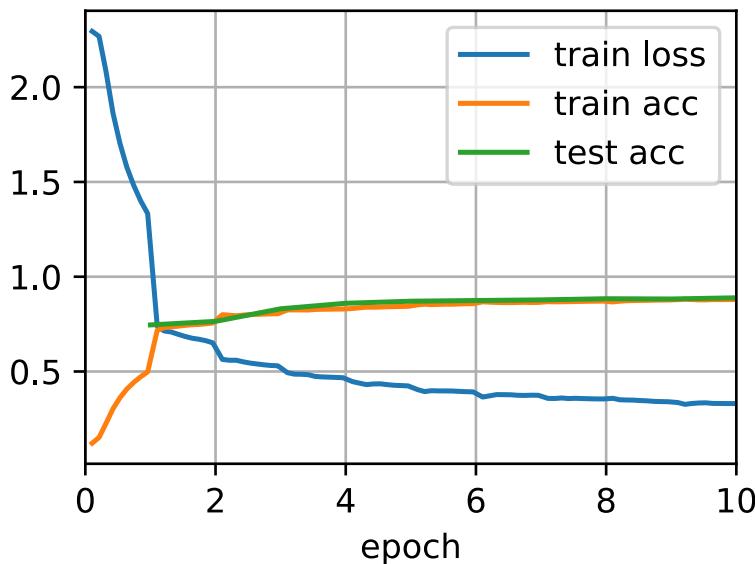
```
batch_size = 128
train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size, resize=224)
```

### 9.1.4 Training

Now, we can start training AlexNet. Compared to LeNet in the previous section, the main change here is the use of a smaller learning rate and much slower training due to the deeper and wider network, the higher image resolution and the more costly convolutions.

```
lr, num_epochs = 0.01, 10
d2l.train_ch5(net, train_iter, test_iter, num_epochs, lr)
```

```
loss 0.330, train acc 0.880, test acc 0.889
4171.0 examples/sec on gpu(0)
```



### 9.1.5 Summary

- AlexNet has a similar structure to that of LeNet, but uses more convolutional layers and a larger parameter space to fit the large-scale data set ImageNet.
- Today AlexNet has been surpassed by much more effective architectures but it is a key step from shallow to deep networks that are used nowadays.
- Although it seems that there are only a few more lines in AlexNet's implementation than in LeNet, it took the academic community many years to embrace this conceptual change and take advantage of its excellent experimental results. This was also due to the lack of efficient computational tools.
- Dropout, ReLU and preprocessing were the other key steps in achieving excellent performance in computer vision tasks.

### 9.1.6 Exercises

1. Try increasing the number of epochs. Compared with LeNet, how are the results different? Why?
2. AlexNet may be too complex for the Fashion-MNIST data set.
  - Try to simplify the model to make the training faster, while ensuring that the accuracy does not drop significantly.
  - Can you design a better model that works directly on  $28 \times 28$  images.
3. Modify the batch size, and observe the changes in accuracy and GPU memory.
4. Rooflines

- What is the dominant part for the memory footprint of AlexNet?
  - What is the dominant part for computation in AlexNet?
  - How about memory bandwidth when computing the results?
5. Apply dropout and ReLU to LeNet5. Does it improve? How about preprocessing?

### 9.1.7 Scan the QR Code to Discuss<sup>119</sup>



## 9.2 Networks Using Blocks (VGG)

While AlexNet proved that deep convolutional neural networks can achieve good results, it didn't offer a general template to guide subsequent researchers in designing new networks. In the following sections, we will introduce several heuristic concepts commonly used to design deep networks.

Progress in this field mirrors that in chip design where engineers went from placing transistors to logical elements to logic blocks. Similarly, the design of neural network architectures had grown progressively more abstract, with researchers moving from thinking in terms of individual neurons to whole layers, and now to blocks, repeating patterns of layers.

The idea of using blocks first emerged from the [Visual Geometry Group<sup>120</sup>](#) (VGG) at Oxford University. In their eponymously-named VGG network, It's easy to implement these repeated structures in code with any modern deep learning framework by using loops and subroutines.

### 9.2.1 VGG Blocks

The basic building block of classic convolutional networks is a sequence of the following layers: (i) a convolutional layer (with padding to maintain the resolution), (ii) a nonlinearity such as a ReLu. One VGG block consists of a sequence of convolutional layers, followed by a max pooling layer for spatial downsampling. In the original VGG paper [54], the authors employed convolutions with  $3 \times 3$  kernels and  $2 \times 2$  max pooling with stride of 2 (halving the resolution after each block). In the code below, we define a function called `vgg_block` to implement one VGG block. The function takes two arguments corresponding to the number of convolutional layers `num_convs` and the number of output channels `num_channels`.

```
import d2l
from mxnet import gluon, nd
from mxnet.gluon import nn

def vgg_block(num_convs, num_channels):
    blk = nn.Sequential()
    for _ in range(num_convs):
```

(continues on next page)

<sup>119</sup> <https://discuss.mxnet.io/t/2354>

<sup>120</sup> <http://www.robots.ox.ac.uk/~vgg/>

(continued from previous page)

```

blk.add(nn.Conv2D(num_channels, kernel_size=3,
                 padding=1, activation='relu'))
blk.add(nn.MaxPool2D(pool_size=2, strides=2))
return blk

```

## 9.2.2 VGG Network

Like AlexNet and LeNet, the VGG Network can be partitioned into two parts: the first consisting mostly of convolutional and pooling layers and a second consisting of fully-connected layers. The convolutional portion of the net connects several `vgg_block` modules in succession. Below, the variable `conv_arch` consists of a list of tuples (one per block), where each contains two values: the number of convolutional layers and the number of output channels, which are precisely the arguments required to call the `vgg_block` function. The fully-connected module is identical to that covered in AlexNet.

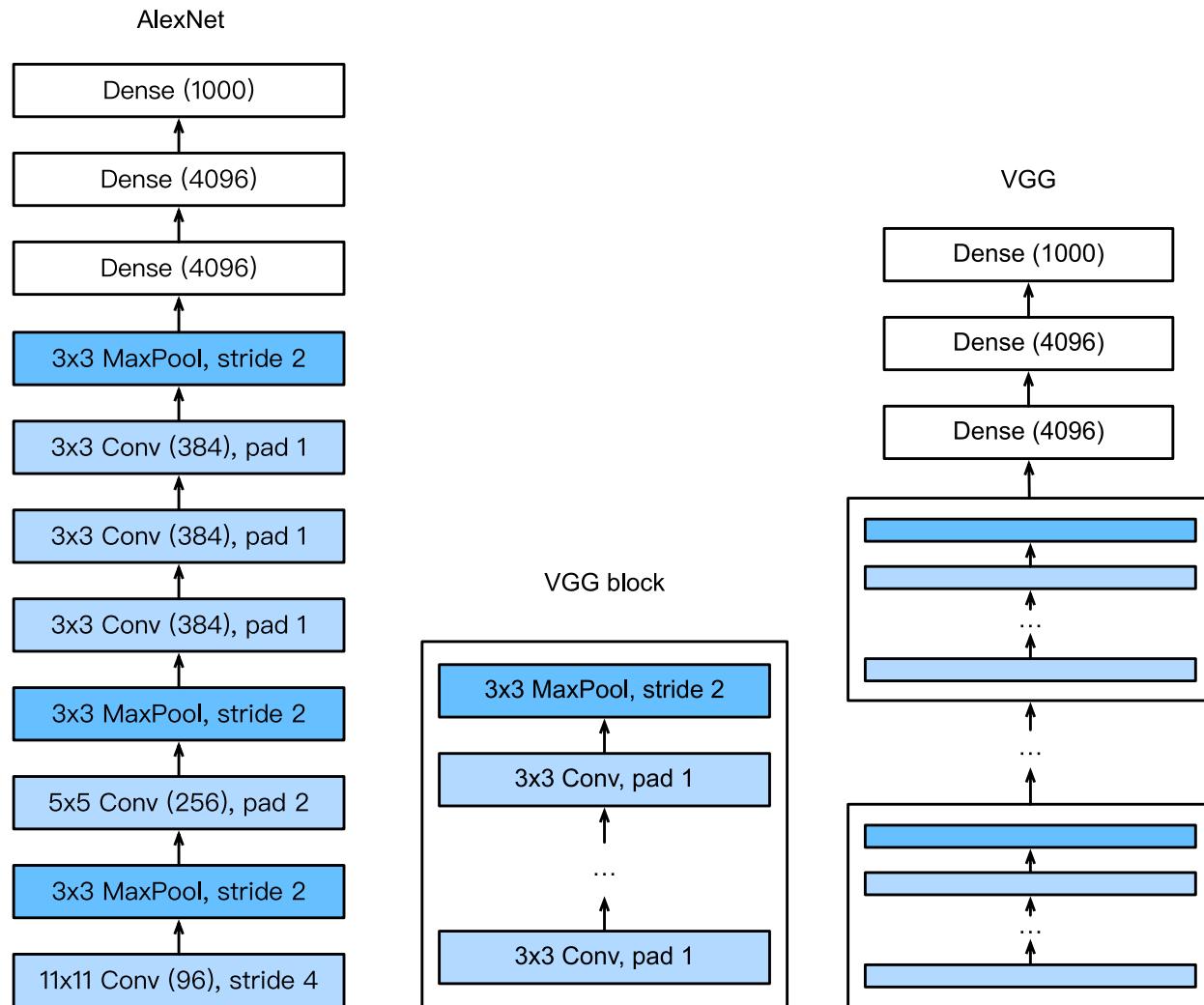


Fig. 9.2.1: Designing a network from building blocks

The original VGG network had 5 convolutional blocks, among which the first two have one convolutional

layer each and the latter three contain two convolutional layers each. The first block has 64 output channels and each subsequent block doubles the number of output channels, until that number reaches 512. Since this network uses 8 convolutional layers and 3 fully-connected layers, it is often called VGG-11.

```
conv_arch = ((1, 64), (1, 128), (2, 256), (2, 512), (2, 512))
```

The following code implements VGG-11. This is a simple matter of executing a for loop over `conv_arch`.

```
def vgg(conv_arch):
    net = nn.Sequential()
    # The convolutional layer part
    for (num_convs, num_channels) in conv_arch:
        net.add(vgg_block(num_convs, num_channels))
    # The fully connected layer part
    net.add(nn.Dense(4096, activation='relu'), nn.Dropout(0.5),
            nn.Dense(4096, activation='relu'), nn.Dropout(0.5),
            nn.Dense(10))
    return net

net = vgg(conv_arch)
```

Next, we will construct a single-channel data example with a height and width of 224 to observe the output shape of each layer.

```
net.initialize()
X = nd.random.uniform(shape=(1, 1, 224, 224))
for blk in net:
    X = blk(X)
    print(blk.name, 'output shape:\t', X.shape)
```

```
sequential1 output shape: (1, 64, 112, 112)
sequential2 output shape: (1, 128, 56, 56)
sequential3 output shape: (1, 256, 28, 28)
sequential4 output shape: (1, 512, 14, 14)
sequential5 output shape: (1, 512, 7, 7)
dense0 output shape: (1, 4096)
dropout0 output shape: (1, 4096)
dense1 output shape: (1, 4096)
dropout1 output shape: (1, 4096)
dense2 output shape: (1, 10)
```

As you can see, we halve height and width at each block, finally reaching a height and width of 7 before flattening the representations for processing by the fully-connected layer.

### 9.2.3 Model Training

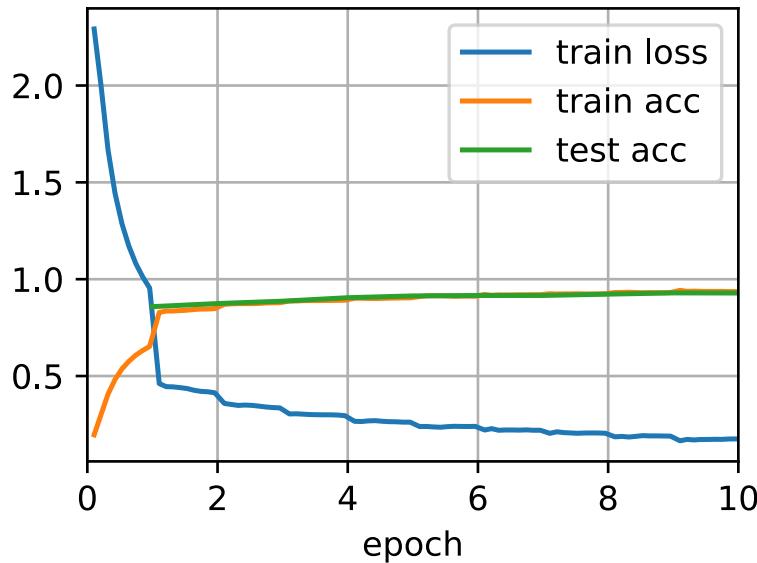
Since VGG-11 is more computationally-heavy than AlexNet we construct a network with a smaller number of channels. This is more than sufficient for training on Fashion-MNIST.

```
ratio = 4
small_conv_arch = [(pair[0], pair[1] // ratio) for pair in conv_arch]
net = vgg(small_conv_arch)
```

Apart from using a slightly larger learning rate, the model training process is similar to that of AlexNet in the last section.

```
lr, num_epochs, batch_size = 0.05, 10, 128,  
train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size, resize=224)  
d2l.train_ch5(net, train_iter, test_iter, num_epochs, lr)
```

```
loss 0.174, train acc 0.936, test acc 0.929  
1796.2 examples/sec on gpu(0)
```



## 9.2.4 Summary

- VGG-11 constructs a network using reusable convolutional blocks. Different VGG models can be defined by the differences in the number of convolutional layers and output channels in each block.
- The use of blocks leads to very compact representations of the network definition. It allows for efficient design of complex networks.
- In their work Simonyan and Ziserman experimented with various architectures. In particular, they found that several layers of deep and narrow convolutions (i.e.  $3 \times 3$ ) were more effective than fewer layers of wider convolutions.

## 9.2.5 Exercises

1. When printing out the dimensions of the layers we only saw 8 results rather than 11. Where did the remaining 3 layer informations go?
2. Compared with AlexNet, VGG is much slower in terms of computation, and it also needs more GPU memory. Try to analyze the reasons for this.
3. Try to change the height and width of the images in Fashion-MNIST from 224 to 96. What influence does this have on the experiments?
4. Refer to Table 1 in [54] to construct other common models, such as VGG-16 or VGG-19.

## 9.2.6 Scan the QR Code to Discuss<sup>121</sup>



## 9.3 Network in Network (NiN)

LeNet, AlexNet, and VGG all share a common design pattern: extract features exploiting *spatial* structure via a sequence of convolutions and pooling layers and then post-process the representations via fully-connected layers. The improvements upon LeNet by AlexNet and VGG mainly lie in how these later networks widen and deepen these two modules. Alternatively, one could imagine using fully-connected layers earlier in the process. However, a careless use of dense layers might give up the spatial structure of the representation entirely, Network in Network (NiN) blocks offer an alternative. They were proposed in [36] based on a very simple insight—to use an MLP on the channels for each pixel separately.

### 9.3.1 NiN Blocks

Recall that the inputs and outputs of convolutional layers consist of four-dimensional arrays with axes corresponding to the batch, channel, height, and width. Also recall that the inputs and outputs of fully-connected layers are typically two-dimensional arrays corresponding to the batch, and features. The idea behind NiN is to apply a fully-connected layer at each pixel location (for each height and width). If we tie the weights across each spatial location, we could think of this as a  $1 \times 1$  convolutional layer (as described in Section 8.4) or as a fully-connected layer acting independently on each pixel location. Another way to view this is to think of each element in the spatial dimension (height and width) as equivalent to an example and the channel as equivalent to a feature. The figure below illustrates the main structural differences between NiN and AlexNet, VGG, and other networks.

The NiN block consists of one convolutional layer followed by two  $1 \times 1$  convolutional layers that act as per-pixel fully-connected layers with ReLU activations. The convolution width of the first layer is typically set by the user. The subsequent widths are fixed to  $1 \times 1$ .

```
import d2l
from mxnet import gluon, nd
from mxnet.gluon import nn

def nin_block(num_channels, kernel_size, strides, padding):
    blk = nn.Sequential()
    blk.add(nn.Conv2D(num_channels, kernel_size, strides, padding, activation='relu'),
           nn.Conv2D(num_channels, kernel_size=1, activation='relu'),
           nn.Conv2D(num_channels, kernel_size=1, activation='relu'))
    return blk
```

<sup>121</sup> <https://discuss.mxnet.io/t/2355>

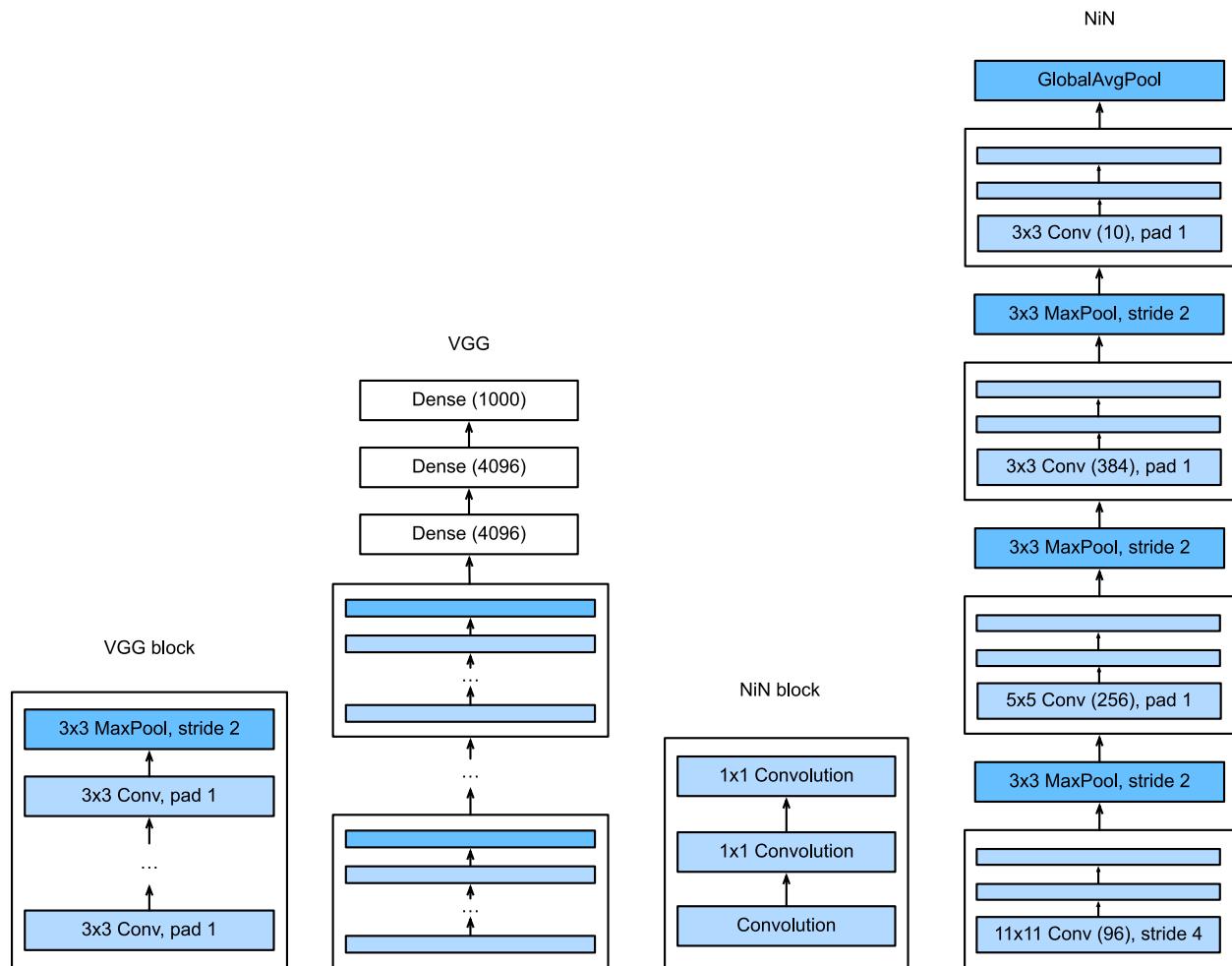


Fig. 9.3.1: The figure on the left shows the network structure of AlexNet and VGG, and the figure on the right shows the network structure of NiN.

### 9.3.2 NiN Model

The original NiN network was proposed shortly after AlexNet and clearly draws some inspiration. NiN uses convolutional layers with window shapes of  $11 \times 11$ ,  $5 \times 5$ , and  $3 \times 3$ , and the corresponding numbers of output channels are the same as in AlexNet. Each NiN block is followed by a maximum pooling layer with a stride of 2 and a window shape of  $3 \times 3$ .

One significant difference between NiN and AlexNet is that NiN avoids dense connections altogether. Instead, NiN uses an NiN block with a number of output channels equal to the number of label classes, followed by a *global* average pooling layer, yielding a vector of logits<sup>122</sup>. One advantage of NiN's design is that it significantly reduces the number of required model parameters. However, in practice, this design sometimes requires increased model training time.

```
net = nn.Sequential()
net.add(nin_block(96, kernel_size=11, strides=4, padding=0),
        nn.MaxPool2D(pool_size=3, strides=2),
        nin_block(256, kernel_size=5, strides=1, padding=2),
        nn.MaxPool2D(pool_size=3, strides=2),
        nin_block(384, kernel_size=3, strides=1, padding=1),
        nn.MaxPool2D(pool_size=3, strides=2),
        nn.Dropout(0.5),
        # There are 10 label classes
        nin_block(10, kernel_size=3, strides=1, padding=1),
        # The global average pooling layer automatically sets the window shape
        # to the height and width of the input
        nn.GlobalAvgPool2D(),
        # Transform the four-dimensional output into two-dimensional output
        # with a shape of (batch size, 10)
        nn.Flatten())
```

We create a data example to see the output shape of each block.

```
X = nd.random.uniform(shape=(1, 1, 224, 224))
net.initialize()
for layer in net:
    X = layer(X)
    print(layer.name, 'output shape:\t', X.shape)
```

```
sequential1 output shape: (1, 96, 54, 54)
pool0 output shape: (1, 96, 26, 26)
sequential2 output shape: (1, 256, 26, 26)
pool1 output shape: (1, 256, 12, 12)
sequential3 output shape: (1, 384, 12, 12)
pool2 output shape: (1, 384, 5, 5)
dropout0 output shape: (1, 384, 5, 5)
sequential4 output shape: (1, 10, 5, 5)
pool3 output shape: (1, 10, 1, 1)
flatten0 output shape: (1, 10)
```

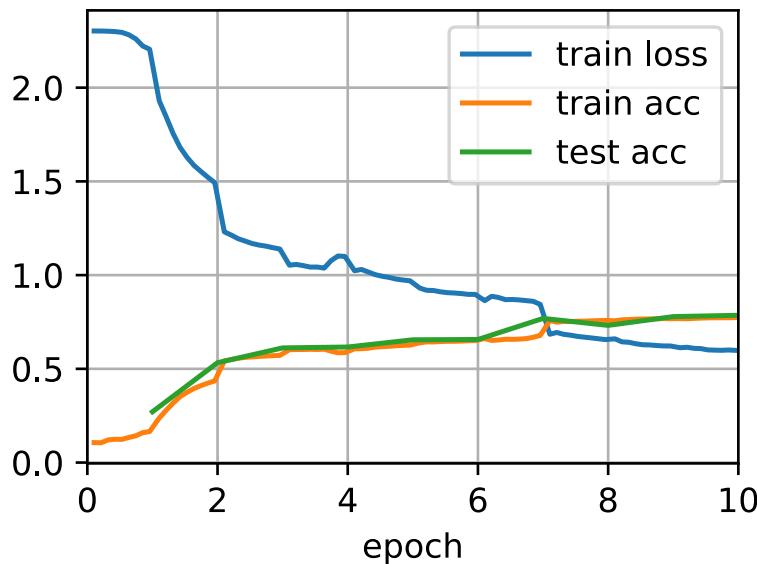
<sup>122</sup> <https://en.wikipedia.org/wiki/Logit>

### 9.3.3 Data Acquisition and Training

As before we use Fashion-MNIST to train the model. NiN's training is similar to that for AlexNet and VGG, but it often uses a larger learning rate.

```
lr, num_epochs, batch_size = 0.1, 10, 128
train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size, resize=224)
d2l.train_ch5(net, train_iter, test_iter, num_epochs, lr)
```

```
loss 0.598, train acc 0.774, test acc 0.786
2962.3 examples/sec on gpu(0)
```



### 9.3.4 Summary

- NiN uses blocks consisting of a convolutional layer and multiple  $1 \times 1$  convolutional layer. This can be used within the convolutional stack to allow for more per-pixel nonlinearity.
- NiN removes the fully connected layers and replaces them with global average pooling (i.e. summing over all locations) after reducing the number of channels to the desired number of outputs (e.g. 10 for Fashion-MNIST).
- Removing the dense layers reduces overfitting. NiN has dramatically fewer parameters.
- The NiN design influenced many subsequent convolutional neural networks designs.

### 9.3.5 Exercises

1. Tune the hyper-parameters to improve the classification accuracy.
2. Why are there two  $1 \times 1$  convolutional layers in the NiN block? Remove one of them, and then observe and analyze the experimental phenomena.
3. Calculate the resource usage for NiN
  - What is the number of parameters?

- What is the amount of computation?
  - What is the amount of memory needed during training?
  - What is the amount of memory needed during inference?
4. What are possible problems with reducing the  $384 \times 5 \times 5$  representation to a  $10 \times 5 \times 5$  representation in one step?

### 9.3.6 Scan the QR Code to Discuss<sup>123</sup>



## 9.4 Networks with Parallel Concatenations (GoogLeNet)

In 2014, [58] won the ImageNet Challenge, proposing a structure that combined the strengths of the NiN and repeated blocks paradigms. One focus of the paper was to address the question of which sized convolutional kernels are best. After all, previous popular networks employed choices as small as  $1 \times 1$  and as large as  $11 \times 11$ . One insight in this paper was that sometimes it can be advantageous to employ a combination of variously-sized kernels. In this section, we will introduce GoogLeNet, presenting a slightly simplified version of the original model—we omit a few ad hoc features that were added to stabilize training but are unnecessary now with better training algorithms available.

### 9.4.1 Inception Blocks

The basic convolutional block in GoogLeNet is called an Inception block, likely named due to a quote from the movie Inception (“We Need To Go Deeper”), which launched a viral meme.

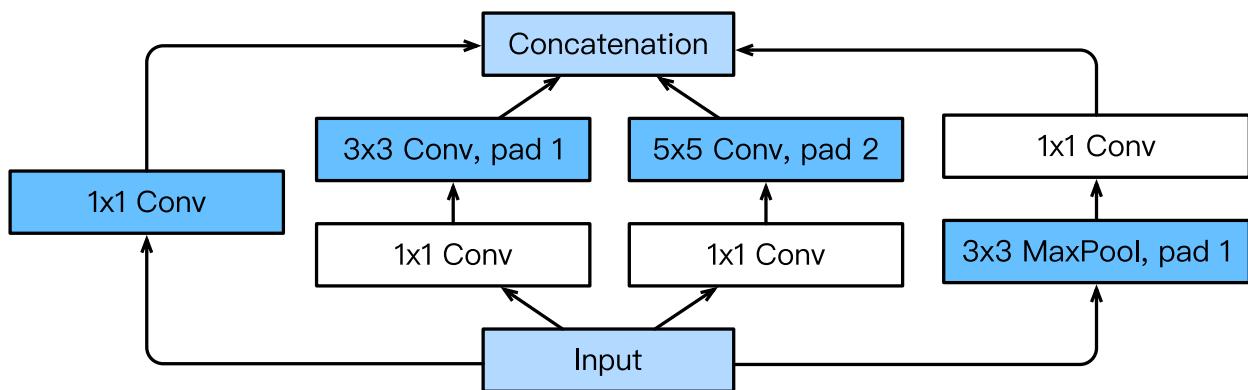


Fig. 9.4.1: Structure of the Inception block.

As depicted in the figure above, the inception block consists of four parallel paths. The first three paths use convolutional layers with window sizes of  $1 \times 1$ ,  $3 \times 3$ , and  $5 \times 5$  to extract information from different spatial

<sup>123</sup> <https://discuss.mxnet.io/t/2356>

sizes. The middle two paths perform a  $1 \times 1$  convolution on the input to reduce the number of input channels, reducing the model's complexity. The fourth path uses a  $3 \times 3$  maximum pooling layer, followed by a  $1 \times 1$  convolutional layer to change the number of channels. The four paths all use appropriate padding to give the input and output the same height and width. Finally, the outputs along each path are concatenated along the channel dimension and comprise the block's output. The commonly-tuned parameters of the Inception block are the number of output channels per layer.

```
import d2l
from mxnet import gluon, nd
from mxnet.gluon import nn

class Inception(nn.Block):
    # c1 - c4 are the number of output channels for each layer in the path
    def __init__(self, c1, c2, c3, c4, **kwargs):
        super(Inception, self).__init__(**kwargs)
        # Path 1 is a single  $1 \times 1$  convolutional layer
        self.p1_1 = nn.Conv2D(c1, kernel_size=1, activation='relu')
        # Path 2 is a  $1 \times 1$  convolutional layer followed by a  $3 \times 3$ 
        # convolutional layer
        self.p2_1 = nn.Conv2D(c2[0], kernel_size=1, activation='relu')
        self.p2_2 = nn.Conv2D(c2[1], kernel_size=3, padding=1,
                             activation='relu')
        # Path 3 is a  $1 \times 1$  convolutional layer followed by a  $5 \times 5$ 
        # convolutional layer
        self.p3_1 = nn.Conv2D(c3[0], kernel_size=1, activation='relu')
        self.p3_2 = nn.Conv2D(c3[1], kernel_size=5, padding=2,
                             activation='relu')
        # Path 4 is a  $3 \times 3$  maximum pooling layer followed by a  $1 \times 1$ 
        # convolutional layer
        self.p4_1 = nn.MaxPool2D(pool_size=3, strides=1, padding=1)
        self.p4_2 = nn.Conv2D(c4, kernel_size=1, activation='relu')

    def forward(self, x):
        p1 = self.p1_1(x)
        p2 = self.p2_2(self.p2_1(x))
        p3 = self.p3_2(self.p3_1(x))
        p4 = self.p4_2(self.p4_1(x))
        # Concatenate the outputs on the channel dimension
        return nd.concat(p1, p2, p3, p4, dim=1)
```

To gain some intuition for why this network works so well, consider the combination of the filters. They explore the image in varying ranges. This means that details at different extents can be recognized efficiently by different filters. At the same time, we can allocate different amounts of parameters for different ranges (e.g. more for short range but not ignore the long range entirely).

### 9.4.2 GoogLeNet Model

GoogLeNet uses a stack of a total of 9 inception blocks and global average pooling to generate its estimates. Maximum pooling between inception blocks reduced the dimensionality. The first part is identical to AlexNet and LeNet, the stack of blocks is inherited from VGG and the global average pooling avoids a stack of fully-connected layers at the end. The architecture is depicted below.

We can now implement GoogLeNet piece by piece. The first component uses a 64-channel  $7 \times 7$  convolutional layer.

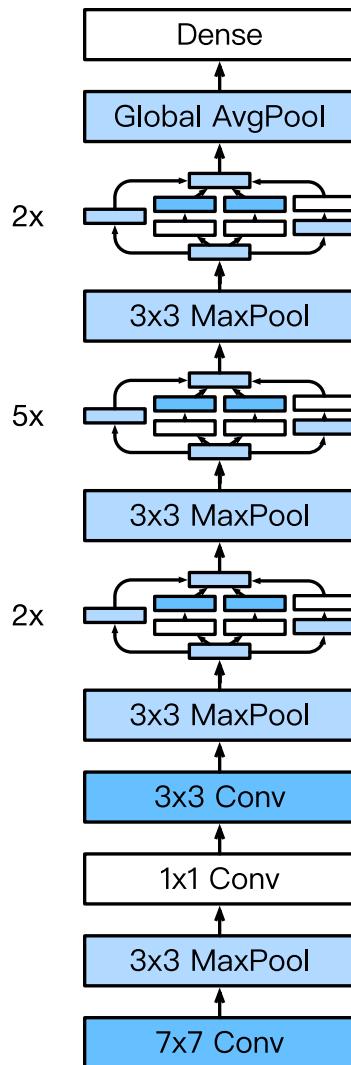


Fig. 9.4.2: Full GoogLeNet Model

```
b1 = nn.Sequential()
b1.add(nn.Conv2D(64, kernel_size=7, strides=2, padding=3, activation='relu'),
       nn.MaxPool2D(pool_size=3, strides=2, padding=1))
```

The second component uses two convolutional layers: first, a 64-channel  $1 \times 1$  convolutional layer, then a  $3 \times 3$  convolutional layer that triples the number of channels. This corresponds to the second path in the Inception block.

```
b2 = nn.Sequential()
b2.add(nn.Conv2D(64, kernel_size=1, activation='relu'),
       nn.Conv2D(192, kernel_size=3, padding=1, activation='relu'),
       nn.MaxPool2D(pool_size=3, strides=2, padding=1))
```

The third component connects two complete Inception blocks in series. The number of output channels of the first Inception block is  $64 + 128 + 32 + 32 = 256$ , and the ratio to the output channels of the four paths is  $64 : 128 : 32 : 32 = 2 : 4 : 1 : 1$ . The second and third paths first reduce the number of input channels to  $96/192 = 1/2$  and  $16/192 = 1/12$ , respectively, and then connect the second convolutional layer. The number of output channels of the second Inception block is increased to  $128 + 192 + 96 + 64 = 480$ , and the ratio to the number of output channels per path is  $128 : 192 : 96 : 64 = 4 : 6 : 3 : 2$ . The second and third paths first reduce the number of input channels to  $128/256 = 1/2$  and  $32/256 = 1/8$ , respectively.

```
b3 = nn.Sequential()
b3.add(Inception(64, (96, 128), (16, 32), 32),
       Inception(128, (128, 192), (32, 96), 64),
       nn.MaxPool2D(pool_size=3, strides=2, padding=1))
```

The fourth block is more complicated. It connects five Inception blocks in series, and they have  $192 + 208 + 48 + 64 = 512$ ,  $160 + 224 + 64 + 64 = 512$ ,  $128 + 256 + 64 + 64 = 512$ ,  $112 + 288 + 64 + 64 = 528$ , and  $256 + 320 + 128 + 128 = 832$  output channels, respectively. The number of channels assigned to these paths is similar to that in the third module: the second path with the  $3 \times 3$  convolutional layer outputs the largest number of channels, followed by the first path with only the  $1 \times 1$  convolutional layer, the third path with the  $5 \times 5$  convolutional layer, and the fourth path with the  $3 \times 3$  maximum pooling layer. The second and third paths will first reduce the number of channels according to the ratio. These ratios are slightly different in different Inception blocks.

```
b4 = nn.Sequential()
b4.add(Inception(192, (96, 208), (16, 48), 64),
       Inception(160, (112, 224), (24, 64), 64),
       Inception(128, (128, 256), (24, 64), 64),
       Inception(112, (144, 288), (32, 64), 64),
       Inception(256, (160, 320), (32, 128), 128),
       nn.MaxPool2D(pool_size=3, strides=2, padding=1))
```

The fifth block has two Inception blocks with  $256 + 320 + 128 + 128 = 832$  and  $384 + 384 + 128 + 128 = 1024$  output channels. The number of channels assigned to each path is the same as that in the third and fourth modules, but differs in specific values. It should be noted that the fifth block is followed by the output layer. This block uses the global average pooling layer to change the height and width of each channel to 1, just as in NiN. Finally, we turn the output into a two-dimensional array followed by a fully-connected layer whose number of outputs is the number of label classes.

```
b5 = nn.Sequential()
b5.add(Inception(256, (160, 320), (32, 128), 128),
       Inception(384, (192, 384), (48, 128), 128),
```

(continues on next page)

(continued from previous page)

```
nn.GlobalAvgPool2D()

net = nn.Sequential()
net.add(b1, b2, b3, b4, b5, nn.Dense(10))
```

The GoogLeNet model is computationally complex, so it is not as easy to modify the number of channels as in VGG. To have a reasonable training time on Fashion-MNIST, we reduce the input height and width from 224 to 96. This simplifies the computation. The changes in the shape of the output between the various modules is demonstrated below.

```
X = nd.random.uniform(shape=(1, 1, 96, 96))
net.initialize()
for layer in net:
    X = layer(X)
    print(layer.name, 'output shape:\t', X.shape)
```

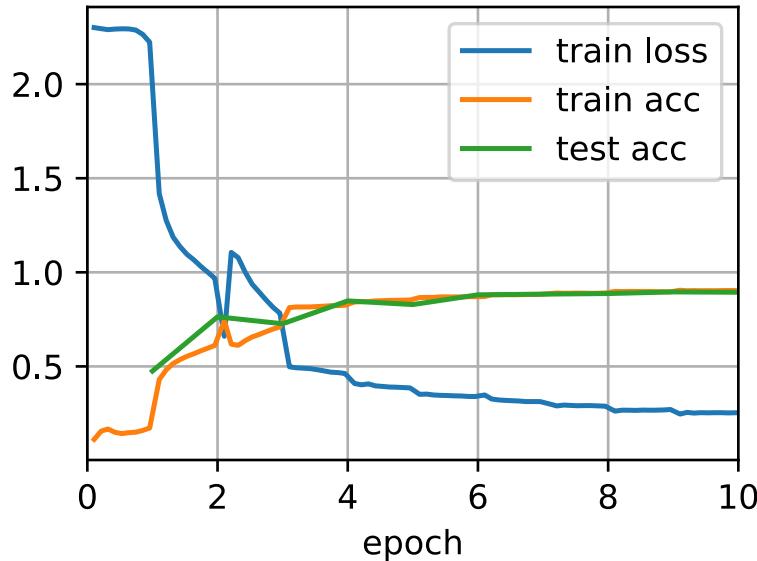
```
sequential0 output shape: (1, 64, 24, 24)
sequential1 output shape: (1, 192, 12, 12)
sequential2 output shape: (1, 480, 6, 6)
sequential3 output shape: (1, 832, 3, 3)
sequential4 output shape: (1, 1024, 1, 1)
dense0 output shape: (1, 10)
```

### 9.4.3 Data Acquisition and Training

As before, we train our model using the Fashion-MNIST dataset. We transform it to  $96 \times 96$  pixel resolution before invoking the training procedure.

```
lr, num_epochs, batch_size = 0.1, 10, 128
train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size, resize=96)
d2l.train_ch5(net, train_iter, test_iter, num_epochs, lr)
```

```
loss 0.254, train acc 0.903, test acc 0.894
2778.9 examples/sec on gpu(0)
```



#### 9.4.4 Summary

- The Inception block is equivalent to a subnetwork with four paths. It extracts information in parallel through convolutional layers of different window shapes and maximum pooling layers.  $1 \times 1$  convolutions reduce channel dimensionality on a per-pixel level. Max-pooling reduces the resolution.
- GoogLeNet connects multiple well-designed Inception blocks with other layers in series. The ratio of the number of channels assigned in the Inception block is obtained through a large number of experiments on the ImageNet data set.
- GoogLeNet, as well as its succeeding versions, was one of the most efficient models on ImageNet, providing similar test accuracy with lower computational complexity.

#### 9.4.5 Exercises

1. There are several iterations of GoogLeNet. Try to implement and run them. Some of them include the following:
  - Add a batch normalization layer [27], as described later in Section 9.5.
  - Make adjustments to the Inception block [59].
  - Use “label smoothing” for model regularization [59].
  - Include it in the residual connection [57], as described later in Section 9.6.
2. What is the minimum image size for GoogLeNet to work?
3. Compare the model parameter sizes of AlexNet, VGG, and NiN with GoogLeNet. How do the latter two network architectures significantly reduce the model parameter size?
4. Why do we need a large range convolution initially?

#### 9.4.6 Scan the QR Code to Discuss<sup>124</sup>

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<sup>124</sup> <https://discuss.mxnet.io/t/2357>



## 9.5 Batch Normalization

Training deep models is difficult and getting them to converge in a reasonable amount of time can be tricky. In this section, we describe batch normalization (BN) [27], one popular and effective technique that has been found to accelerate the convergence of deep nets, and together with residual blocks, which we cover in Section 9.6, has recently enabled practitioners to routinely train networks with over 100 layers.

### 9.5.1 Training Deep Networks

Let's review some of the practical challenges when training deep networks.

1. Data preprocessing often proves to be a crucial consideration for effective statistical modeling. Recall our application of deep networks to predicting house prices in Section 6.10. In that example, we standardized our input features to each have a mean of *zero* and variance of *one*. Standardizing input data typically makes it easier to train models since parameters are a-priori at a similar scale.
2. For a typical MLP or CNN, as we train the model, the activations in intermediate layers of the network may assume different orders of magnitude (both across nodes in the same layer, and over time due to updating the model's parameters). The authors of the batch normalization technique postulated that this drift in the distribution of activations could hamper the convergence of the network. Intuitively, we might conjecture that if one layer has activation values that are 100x that of another layer, we might need to adjust learning rates adaptively per layer (or even per node within a layer).
3. Deeper networks are complex and easily capable of overfitting. This means that regularization becomes more critical. Empirically, we note that even with dropout, models can overfit badly and we might benefit from other regularization heuristics.

In 2015, a clever heuristic called batch normalization (BN) that has proved immensely useful for improving the reliability and speed of convergence when training deep models [27]. In each training iteration, BN normalizes the activations of each hidden layer node (on each layer where it is applied) by subtracting its mean and dividing by its standard deviation, estimating both based on the current minibatch. Note that if our batch size was 1, we wouldn't be able to learn anything because during training, every hidden node would take value 0. However, with large enough minibatches, the approach proves effective and stable.

In a nutshell, the idea in Batch Normalization is to transform the activation at a given layer from  $\mathbf{x}$  to

$$\text{BN}(\mathbf{x}) = \gamma \odot \frac{\mathbf{x} - \hat{\mu}}{\hat{\sigma}} + \beta \quad (9.5.1)$$

Here,  $\hat{\mu}$  is the estimate of the mean and  $\hat{\sigma}$  is the estimate of the variance. The result is that the activations are approximately rescaled to zero mean and unit variance. Since this may not be quite what we want, we allow for a coordinate-wise scaling coefficient  $\gamma$  and an offset  $\beta$ . Consequently, the activations for intermediate layers cannot diverge any longer: we are actively rescaling them back to a given order of magnitude via  $\mu$  and  $\sigma$ . Intuitively, it is hoped that this normalization allows us to be more aggressive in picking large learning rates. To address the fact that in some cases the activations may actually *need* to differ from standardized data, BN also introduces scaling coefficients  $\gamma$  and an offset  $\beta$ .

In principle, we might want to use all of our training data to estimate the mean and variance. However, the activations corresponding to each example change each time we update our model. To remedy this problem, BN uses only the current minibatch for estimating  $\hat{\mu}$  and  $\hat{\sigma}$ . It is precisely due to this fact that we normalize based only on the *current batch* that *batch normalization* derives its name. To indicate which minibatch  $\mathcal{B}$  we draw from, we denote the quantities with  $\hat{\mu}_{\mathcal{B}}$  and  $\hat{\sigma}_{\mathcal{B}}$ .

$$\hat{\mu}_{\mathcal{B}} \leftarrow \frac{1}{|\mathcal{B}|} \sum_{\mathbf{x} \in \mathcal{B}} \mathbf{x} \text{ and } \hat{\sigma}_{\mathcal{B}}^2 \leftarrow \frac{1}{|\mathcal{B}|} \sum_{\mathbf{x} \in \mathcal{B}} (\mathbf{x} - \hat{\mu}_{\mathcal{B}})^2 + \epsilon \quad (9.5.2)$$

Note that we add a small constant  $\epsilon > 0$  to the variance estimate to ensure that we never end up dividing by zero, even in cases where the empirical variance estimate might vanish by accident. The estimates  $\hat{\mu}_{\mathcal{B}}$  and  $\hat{\sigma}_{\mathcal{B}}$  counteract the scaling issue by using unbiased but noisy estimates of mean and variance. Normally we would consider this a problem. After all, each minibatch has different data, different labels and with it, different activations, predictions and errors. As it turns out, this is actually beneficial. This natural variation appears to act as a form of regularization, conferring benefits (as observed empirically) in mitigating overfitting. In other recent preliminary research, [60] and [43] relate the properties of BN to Bayesian Priors and penalties respectively. In particular, this sheds some light on the puzzle why BN works best for moderate sizes of minibatches in the range 50-100.

We are now ready to take a look at how batch normalization works in practice.

## 9.5.2 Batch Normalization Layers

The batch normalization methods for fully-connected layers and convolutional layers are slightly different. This is due to the dimensionality of the data generated by convolutional layers. We discuss both cases below. Note that one of the key differences between BN and other layers is that BN operates on a full minibatch at a time (otherwise it cannot compute the mean and variance parameters per batch).

### Fully-Connected Layers

Usually we apply the batch normalization layer between the affine transformation and the activation function in a fully-connected layer. In the following, we denote by  $\mathbf{u}$  the input and by  $\mathbf{x} = \mathbf{W}\mathbf{u} + \mathbf{b}$  the output of the linear transform. This yields the following variant of BN:

$$\mathbf{y} = \phi(\text{BN}(\mathbf{x})) = \phi(\text{BN}(\mathbf{W}\mathbf{u} + \mathbf{b})) \quad (9.5.3)$$

Recall that mean and variance are computed on the *same* minibatch  $\mathcal{B}$  on which the transformation is applied. Also recall that the scaling coefficient  $\gamma$  and the offset  $\beta$  are parameters that need to be learned. They ensure that the effect of batch normalization can be neutralized as needed.

### Convolutional Layers

For convolutional layers, batch normalization occurs after the convolution computation and before the application of the activation function. If the convolution computation outputs multiple channels, we need to carry out batch normalization for *each* of the outputs of these channels, and each channel has an independent scale parameter and shift parameter, both of which are scalars. Assume that there are  $m$  examples in the mini-batch. On a single channel, we assume that the height and width of the convolution computation output are  $p$  and  $q$ , respectively. We need to carry out batch normalization for  $m \times p \times q$  elements in this channel simultaneously. While carrying out the standardization computation for these elements, we use the same mean and variance. In other words, we use the means and variances of the  $m \times p \times q$  elements in this channel rather than one per pixel.

## Batch Normalization During Prediction

At prediction time, we might not have the luxury of computing offsets per batch—we might be required to make one prediction at a time. Secondly, the uncertainty in  $\mu$  and  $\sigma$ , as arising from a minibatch are undesirable once we've trained the model. One way to mitigate this is to compute more stable estimates on a larger set for once (e.g. via a moving average) and then fix them at prediction time. Consequently, BN behaves differently during training and at test time (recall that dropout also behaves differently at train and test times).

### 9.5.3 Implementation from Scratch

Next, we will implement the batch normalization layer with NDArray from scratch:

```
import d2l
from mxnet import autograd, gluon, nd, init
from mxnet.gluon import nn

def batch_norm(X, gamma, beta, moving_mean, moving_var, eps, momentum):
    # Use autograd to determine whether the current mode is training mode or
    # prediction mode
    if not autograd.is_training():
        # If it is the prediction mode, directly use the mean and variance
        # obtained from the incoming moving average
        X_hat = (X - moving_mean) / nd.sqrt(moving_var + eps)
    else:
        assert len(X.shape) in (2, 4)
        if len(X.shape) == 2:
            # When using a fully connected layer, calculate the mean and
            # variance on the feature dimension
            mean = X.mean(axis=0)
            var = ((X - mean) ** 2).mean(axis=0)
        else:
            # When using a two-dimensional convolutional layer, calculate the
            # mean and variance on the channel dimension (axis=1). Here we
            # need to maintain the shape of X, so that the broadcast operation
            # can be carried out later
            mean = X.mean(axis=(0, 2, 3), keepdims=True)
            var = ((X - mean) ** 2).mean(axis=(0, 2, 3), keepdims=True)
        # In training mode, the current mean and variance are used for the
        # standardization
        X_hat = (X - mean) / nd.sqrt(var + eps)
        # Update the mean and variance of the moving average
        moving_mean = momentum * moving_mean + (1.0 - momentum) * mean
        moving_var = momentum * moving_var + (1.0 - momentum) * var
    Y = gamma * X_hat + beta # Scale and shift
    return Y, moving_mean, moving_var
```

Now, we can customize a `BatchNorm` layer. This retains the scale parameter `gamma` and the shift parameter `beta` involved in gradient finding and iteration, and it also maintains the mean and variance obtained from the moving average, so that they can be used during model prediction. The `num_features` parameter required by the `BatchNorm` instance is the number of outputs for a fully-connected layer and the number of output channels for a convolutional layer. The `num_dims` parameter also required by this instance is 2 for a fully-connected layer and 4 for a convolutional layer.

Besides the algorithm per se, also note the design pattern in implementing layers. Typically one defines the math in a separate function, say `batch_norm`. This is then integrated into a custom layer that mostly focuses on bookkeeping, such as moving data to the right device context, ensuring that variables are properly initialized, keeping track of the running averages for mean and variance, etc. That way we achieve a clean separation of math and boilerplate code. Also note that for the sake of convenience we did not add automagic size inference here, hence we will need to specify the number of features throughout (the Gluon version will take care of this for us).

```
class BatchNorm(nn.Block):
    def __init__(self, num_features, num_dims, **kwargs):
        super(BatchNorm, self).__init__(**kwargs)
        if num_dims == 2:
            shape = (1, num_features)
        else:
            shape = (1, num_features, 1, 1)
        # The scale parameter and the shift parameter involved in gradient
        # finding and iteration are initialized to 0 and 1 respectively
        self.gamma = self.params.get('gamma', shape=shape, init=init.One())
        self.beta = self.params.get('beta', shape=shape, init=init.Zero())
        # All the variables not involved in gradient finding and iteration are
        # initialized to 0 on the CPU
        self.moving_mean = nd.zeros(shape)
        self.moving_var = nd.zeros(shape)

    def forward(self, X):
        # If X is not on the CPU, copy moving_mean and moving_var to the
        # device where X is located
        if self.moving_mean.context != X.context:
            self.moving_mean = self.moving_mean.copyto(X.context)
            self.moving_var = self.moving_var.copyto(X.context)
        # Save the updated moving_mean and moving_var
        Y, self.moving_mean, self.moving_var = batch_norm(
            X, self.gamma.data(), self.beta.data(), self.moving_mean,
            self.moving_var, eps=1e-5, momentum=0.9)
        return Y
```

#### 9.5.4 Use a Batch Normalization LeNet

Next, we will modify the LeNet model (Section 8.6) in order to apply the batch normalization layer. We add the batch normalization layer after all the convolutional layers and after all fully-connected layers. As discussed, we add it before the activation layer.

```
net = nn.Sequential()
net.add(nn.Conv2D(6, kernel_size=5),
       BatchNorm(6, num_dims=4),
       nn.Activation('sigmoid'),
       nn.MaxPool2D(pool_size=2, strides=2),
       nn.Conv2D(16, kernel_size=5),
       BatchNorm(16, num_dims=4),
       nn.Activation('sigmoid'),
       nn.MaxPool2D(pool_size=2, strides=2),
       nn.Dense(120),
```

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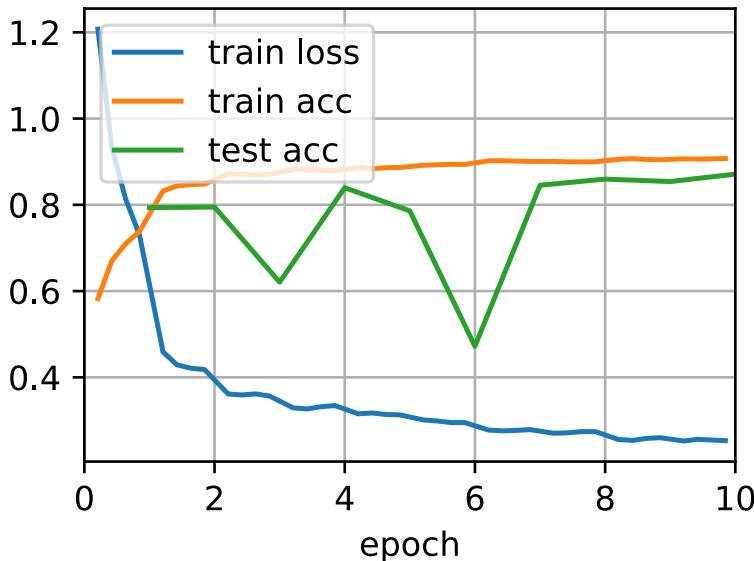
(continued from previous page)

```
BatchNorm(120, num_dims=2),
nn.Activation('sigmoid'),
nn.Dense(84),
BatchNorm(84, num_dims=2),
nn.Activation('sigmoid'),
nn.Dense(10))
```

Next we train the modified model, again on Fashion-MNIST. The code is virtually identical to that in previous steps. The main difference is the considerably larger learning rate.

```
lr, num_epochs, batch_size = 1.0, 10, 256
train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size)
d2l.train_ch5(net, train_iter, test_iter, num_epochs, lr)
```

```
loss 0.253, train acc 0.908, test acc 0.871
24269.4 examples/sec on gpu(0)
```



Let's have a look at the scale parameter `gamma` and the shift parameter `beta` learned from the first batch normalization layer.

```
net[1].gamma.data().reshape((-1,)), net[1].beta.data().reshape((-1,))
```

```
(  
[2.0343778 1.5818421 2.7213738 0.83559245 1.3956174 2.7034783 ]  
<NDArray 6 @gpu(0)>,  
[ 1.1638958 -0.37698063 -0.26598477 0.548655 -0.9186371 -2.8301313 ]  
<NDArray 6 @gpu(0)>)
```

## 9.5.5 Concise Implementation

Compared with the `BatchNorm` class, which we just defined ourselves, the `BatchNorm` class defined by the `nn` model in Gluon is easier to use. In Gluon, we do not have to define the `num_features` and `num_dims` parameters.

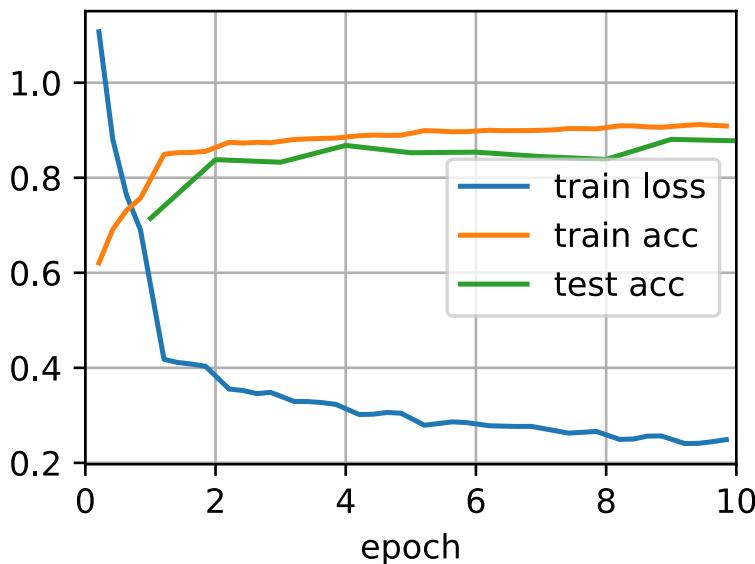
eter values required in the `BatchNorm` class. Instead, these parameter values will be obtained automatically by delayed initialization. The code looks virtually identical (save for the lack of an explicit specification of the dimensionality of the features for the Batch Normalization layers).

```
net = nn.Sequential()
net.add(nn.Conv2D(6, kernel_size=5),
       nn.BatchNorm(),
       nn.Activation('sigmoid'),
       nn.MaxPool2D(pool_size=2, strides=2),
       nn.Conv2D(16, kernel_size=5),
       nn.BatchNorm(),
       nn.Activation('sigmoid'),
       nn.MaxPool2D(pool_size=2, strides=2),
       nn.Dense(120),
       nn.BatchNorm(),
       nn.Activation('sigmoid'),
       nn.Dense(84),
       nn.BatchNorm(),
       nn.Activation('sigmoid'),
       nn.Dense(10))
```

Use the same hyper-parameter to carry out the training. Note that as usual, the Gluon variant runs much faster since its code has been compiled to C++/CUDA vs our custom implementation, which must be interpreted by Python.

```
d2l.train_ch5(net, train_iter, test_iter, num_epochs, lr)
```

```
loss 0.249, train acc 0.909, test acc 0.878
52761.1 examples/sec on gpu(0)
```



### 9.5.6 Controversy

Intuitively, batch normalization is thought to somehow make the optimization landscape smoother. However, we must be careful to distinguish between speculative intuitions and true explanations for the phenomena that we observe when training deep models. Recall that we do not even know why simpler deep neural networks (MLPs and conventional CNNs) generalize so well. Despite dropout and L2 regularization, they remain too flexible to admit conventional learning-theoretic generalization guarantees.

In the original paper proposing batch normalization, the authors, in addition to introducing a powerful and useful tool offered an explanation for why it works: by reducing *internal covariate shift*. Presumably by *internal covariate shift* the authors meant something like the intuition expressed above—the notion that the distribution of activations changes over the course of training. However there were two problems with this explanation: (1) This drift is very different from *covariate shift*, rendering the name a misnomer. (2) The explanation remains ill-defined (and thus unproven)—rendering *why precisely this technique works* an open question. Throughout this book we aim to convey the intuitions that practitioners use to guide their development of deep neural networks. However, it's important to separate these guiding heuristics from established scientific fact. Eventually, when you master this material and start writing your own research papers you will want to be clear to delineate between technical claims and hunches.

Following the success of batch normalization, its explanation and via *internal covariate shift* became a hot topic that has been revisited several times both in the technical literature and in the broader discourse about how machine learning research ought to be presented. Ali Rahimi popularly raised this issue during a memorable speech while accepting a Test of Time Award at the NeurIPS conference in 2017 and the issue was revisited in a recent position paper on troubling trends in machine learning [39]. In the technical literature other authors ([52]) have proposed alternative explanations for the success of BN, some claiming that BN's success comes despite exhibiting behavior that is in some ways opposite to those claimed in the original paper.

### 9.5.7 Summary

- During model training, batch normalization continuously adjusts the intermediate output of the neural network by utilizing the mean and standard deviation of the mini-batch, so that the values of the intermediate output in each layer throughout the neural network are more stable.
- The batch normalization methods for fully connected layers and convolutional layers are slightly different.
- Like a dropout layer, batch normalization layers have different computation results in training mode and prediction mode.
- Batch Normalization has many beneficial side effects, primarily that of regularization. On the other hand, the original motivation of reducing covariate shift seems not to be a valid explanation.

### 9.5.8 Exercises

1. Can we remove the fully connected affine transformation before the batch normalization or the bias parameter in convolution computation?
  - Find an equivalent transformation that applies prior to the fully connected layer.
  - Is this reformulation effective. Why (not)?
2. Compare the learning rates for LeNet with and without batch normalization.
  - Plot the decrease in training and test error.
  - What about the region of convergence? How large can you make the learning rate?

3. Do we need Batch Normalization in every layer? Experiment with it?
4. Can you replace Dropout by Batch Normalization? How does the behavior change?
5. Fix the coefficients `beta` and `gamma` (add the parameter `grad_req='null'` at the time of construction to avoid calculating the gradient), and observe and analyze the results.
6. Review the Gluon documentation for `BatchNorm` to see the other applications for Batch Normalization.
7. Research ideas - think of other normalization transforms that you can apply? Can you apply the probability integral transform? How about a full rank covariance estimate?

### 9.5.9 Scan the QR Code to Discuss<sup>125</sup>



## 9.6 Residual Networks (ResNet)

As we design increasingly deeper networks it becomes imperative to understand how adding layers can increase the complexity and expressiveness of the network. Even more important is the ability to design networks where adding layers makes networks strictly more expressive rather than just different. To make some progress we need a bit of theory.

### 9.6.1 Function Classes

Consider  $\mathcal{F}$ , the class of functions that a specific network architecture (together with learning rates and other hyperparameter settings) can reach. That is, for all  $f \in \mathcal{F}$  there exists some set of parameters  $W$  that can be obtained through training on a suitable dataset. Let's assume that  $f^*$  is the function that we really would like to find. If it's in  $\mathcal{F}$ , we're in good shape but typically we won't be quite so lucky. Instead, we will try to find some  $f_{\mathcal{F}}^*$  which is our best bet within  $\mathcal{F}$ . For instance, we might try finding it by solving the following optimization problem:

$$f_{\mathcal{F}}^* := \underset{f}{\operatorname{argmin}} L(X, Y, f) \text{ subject to } f \in \mathcal{F} \quad (9.6.1)$$

It is only reasonable to assume that if we design a different and more powerful architecture  $\mathcal{F}'$  we should arrive at a better outcome. In other words, we would expect that  $f_{\mathcal{F}'}^*$  is 'better' than  $f_{\mathcal{F}}^*$ . However, if  $\mathcal{F} \not\subseteq \mathcal{F}'$  there is no guarantee that this should even happen. In fact,  $f_{\mathcal{F}'}^*$  might well be worse. This is a situation that we often encounter in practice - adding layers doesn't only make the network more expressive, it also changes it in sometimes not quite so predictable ways. The picture below illustrates this in slightly abstract terms.

Only if larger function classes contain the smaller ones are we guaranteed that increasing them strictly increases the expressive power of the network. This is the question that He et al, 2016 considered when working on very deep computer vision models. At the heart of ResNet is the idea that every additional layer should contain the identity function as one of its elements. This means that if we can train the newly-added layer into an identity mapping  $f(\mathbf{x}) = \mathbf{x}$ , the new model will be as effective as the original model. As the new

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<sup>125</sup> <https://discuss.mxnet.io/t/2358>

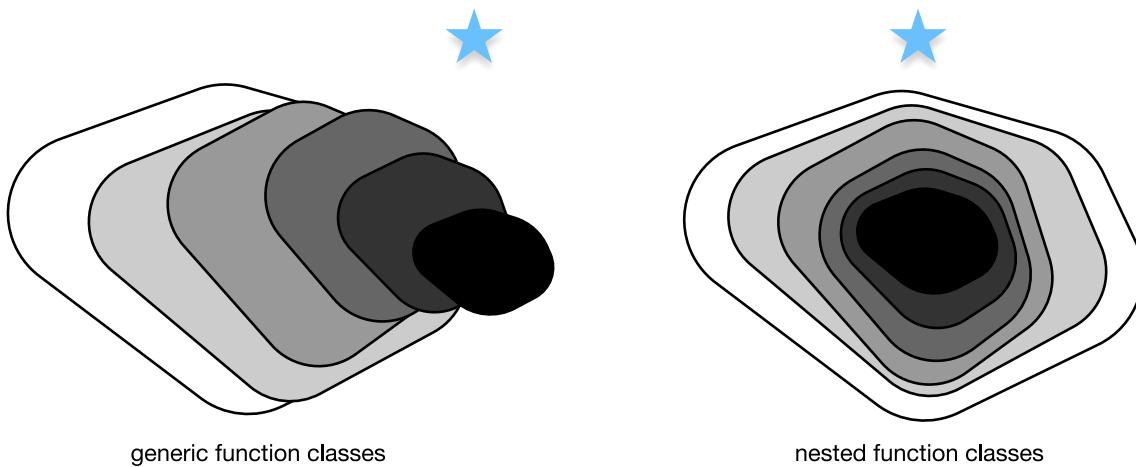


Fig. 9.6.1: Left: non-nested function classes. The distance may in fact increase as the complexity increases. Right: with nested function classes this does not happen.

model may get a better solution to fit the training data set, the added layer might make it easier to reduce training errors. Even better, the identity function rather than the null  $f(\mathbf{x}) = 0$  should be the simplest function within a layer.

These considerations are rather profound but they led to a surprisingly simple solution, a residual block. With it, [22] won the ImageNet Visual Recognition Challenge in 2015. The design had a profound influence on how to build deep neural networks.

## 9.6.2 Residual Blocks

Let us focus on a local neural network, as depicted below. Denote the input by  $\mathbf{x}$ . We assume that the ideal mapping we want to obtain by learning is  $f(\mathbf{x})$ , to be used as the input to the activation function. The portion within the dotted-line box in the left image must directly fit the mapping  $f(\mathbf{x})$ . This can be tricky if we don't need that particular layer and we would much rather retain the input  $\mathbf{x}$ . The portion within the dotted-line box in the right image now only needs to parametrize the *deviation* from the identity, since we return  $\mathbf{x} + f(\mathbf{x})$ . In practice, the residual mapping is often easier to optimize. We only need to set  $f(\mathbf{x}) = 0$ . The right image in the figure below illustrates the basic Residual Block of ResNet. Similar architectures were later proposed for sequence models which we will study later.

ResNet follows VGG's full  $3 \times 3$  convolutional layer design. The residual block has two  $3 \times 3$  convolutional layers with the same number of output channels. Each convolutional layer is followed by a batch normalization layer and a ReLU activation function. Then, we skip these two convolution operations and add the input directly before the final ReLU activation function. This kind of design requires that the output of the two convolutional layers be of the same shape as the input, so that they can be added together. If we want to change the number of channels or the stride, we need to introduce an additional  $1 \times 1$  convolutional layer to transform the input into the desired shape for the addition operation. Let's have a look at the code below.

```
import d2l
from mxnet import gluon, nd
from mxnet.gluon import nn

# Save to the d2l package.
class Residual(nn.Block):
    def __init__(self, num_channels, use_1x1conv=False, strides=1, **kwargs):
```

(continues on next page)

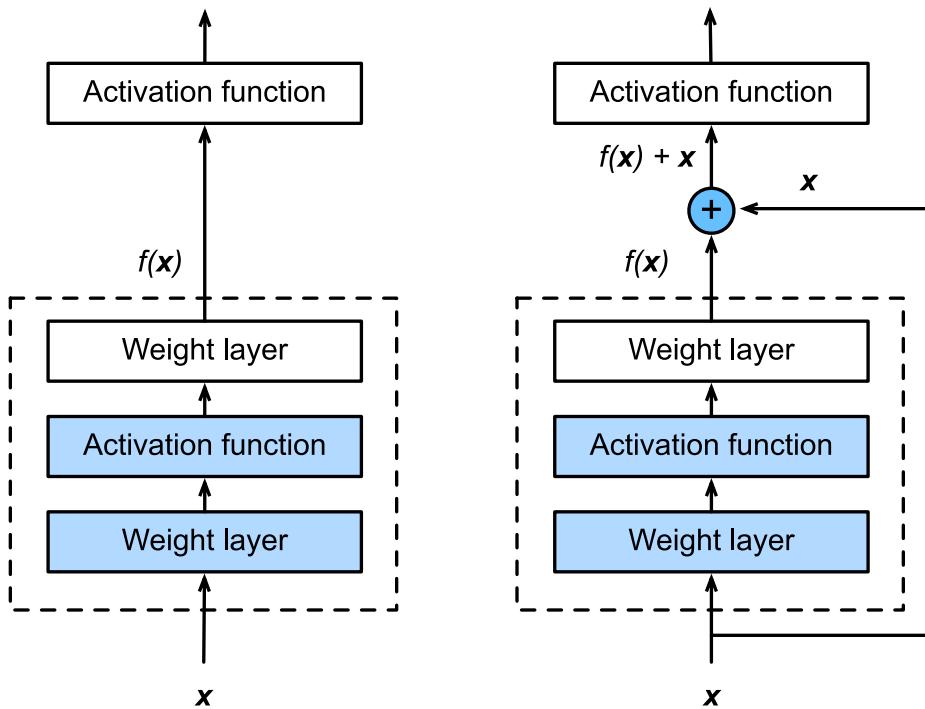


Fig. 9.6.2: The difference between a regular block (left) and a residual block (right). In the latter case, we can short-circuit the convolutions.

(continued from previous page)

```

super(Residual, self).__init__(**kwargs)
self.conv1 = nn.Conv2D(num_channels, kernel_size=3, padding=1,
                     strides=strides)
self.conv2 = nn.Conv2D(num_channels, kernel_size=3, padding=1)
if use_1x1conv:
    self.conv3 = nn.Conv2D(num_channels, kernel_size=1,
                         strides=strides)
else:
    self.conv3 = None
self.bn1 = nn.BatchNorm()
self.bn2 = nn.BatchNorm()

def forward(self, X):
    Y = nd.relu(self.bn1(self.conv1(X)))
    Y = self.bn2(self.conv2(Y))
    if self.conv3:
        X = self.conv3(X)
    return nd.relu(Y + X)

```

This code generates two types of networks: one where we add the input to the output before applying the ReLU nonlinearity, and whenever `use_1x1conv=True`, one where we adjust channels and resolution by means of a  $1 \times 1$  convolution before adding. The diagram below illustrates this:

Now let us look at a situation where the input and output are of the same shape.

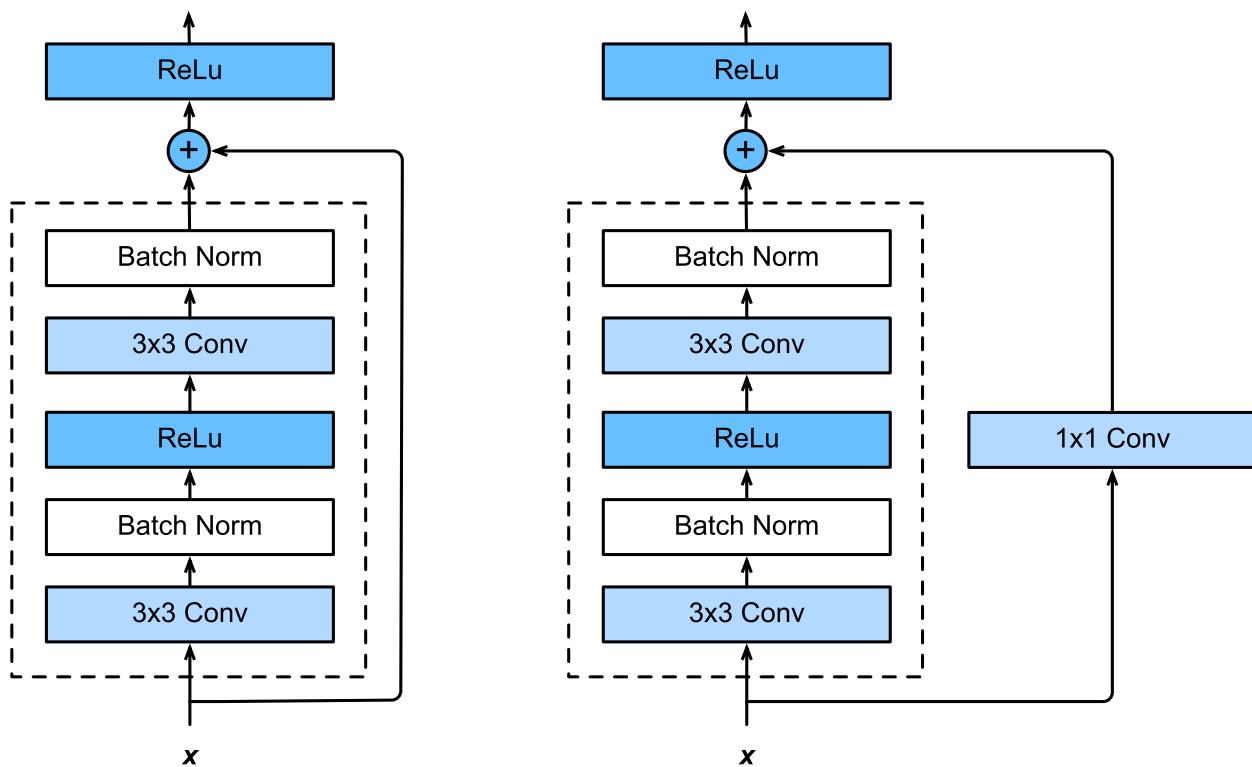


Fig. 9.6.3: Left: regular ResNet block; Right: ResNet block with 1x1 convolution

```
blk = Residual(3)
blk.initialize()
X = nd.random.uniform(shape=(4, 3, 6, 6))
blk(X).shape
```

```
(4, 3, 6, 6)
```

We also have the option to halve the output height and width while increasing the number of output channels.

```
blk = Residual(6, use_1x1conv=True, strides=2)
blk.initialize()
blk(X).shape
```

```
(4, 6, 3, 3)
```

### 9.6.3 ResNet Model

The first two layers of ResNet are the same as those of the GoogLeNet we described before: the  $7 \times 7$  convolutional layer with 64 output channels and a stride of 2 is followed by the  $3 \times 3$  maximum pooling layer with a stride of 2. The difference is the batch normalization layer added after each convolutional layer in ResNet.

```
net = nn.Sequential()
net.add(nn.Conv2D(64, kernel_size=7, strides=2, padding=3),
        nn.BatchNorm(), nn.Activation('relu'),
        nn.MaxPool2D(pool_size=3, strides=2, padding=1))
```

GoogLeNet uses four blocks made up of Inception blocks. However, ResNet uses four modules made up of residual blocks, each of which uses several residual blocks with the same number of output channels. The number of channels in the first module is the same as the number of input channels. Since a maximum pooling layer with a stride of 2 has already been used, it is not necessary to reduce the height and width. In the first residual block for each of the subsequent modules, the number of channels is doubled compared with that of the previous module, and the height and width are halved.

Now, we implement this module. Note that special processing has been performed on the first module.

```
def resnet_block(num_channels, num_residuals, first_block=False):
    blk = nn.Sequential()
    for i in range(num_residuals):
        if i == 0 and not first_block:
            blk.add(Residual(num_channels, use_1x1conv=True, strides=2))
        else:
            blk.add(Residual(num_channels))
    return blk
```

Then, we add all the residual blocks to ResNet. Here, two residual blocks are used for each module.

```
net.add(resnet_block(64, 2, first_block=True),
        resnet_block(128, 2),
        resnet_block(256, 2),
        resnet_block(512, 2))
```

Finally, just like GoogLeNet, we add a global average pooling layer, followed by the fully connected layer output.

```
net.add(nn.GlobalAvgPool2D(), nn.Dense(10))
```

There are 4 convolutional layers in each module (excluding the  $1 \times 1$  convolutional layer). Together with the first convolutional layer and the final fully connected layer, there are 18 layers in total. Therefore, this model is commonly known as ResNet-18. By configuring different numbers of channels and residual blocks in the module, we can create different ResNet models, such as the deeper 152-layer ResNet-152. Although the main architecture of ResNet is similar to that of GoogLeNet, ResNet's structure is simpler and easier to modify. All these factors have resulted in the rapid and widespread use of ResNet. Below is a diagram of the full ResNet-18.

Before training ResNet, let us observe how the input shape changes between different modules in ResNet. As in all previous architectures, the resolution decreases while the number of channels increases up until the point where a global average pooling layer aggregates all features.

```
X = nd.random.uniform(shape=(1, 1, 224, 224))
net.initialize()
for layer in net:
    X = layer(X)
    print(layer.name, 'output shape:\t', X.shape)
```

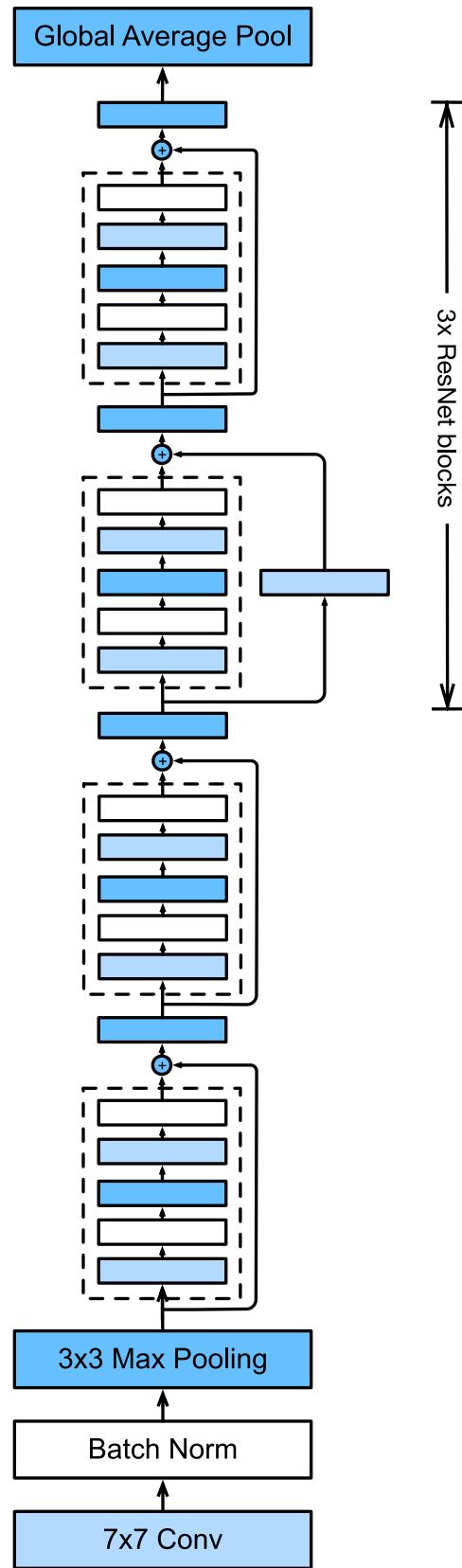


Fig. 9.6.4: ResNet 18

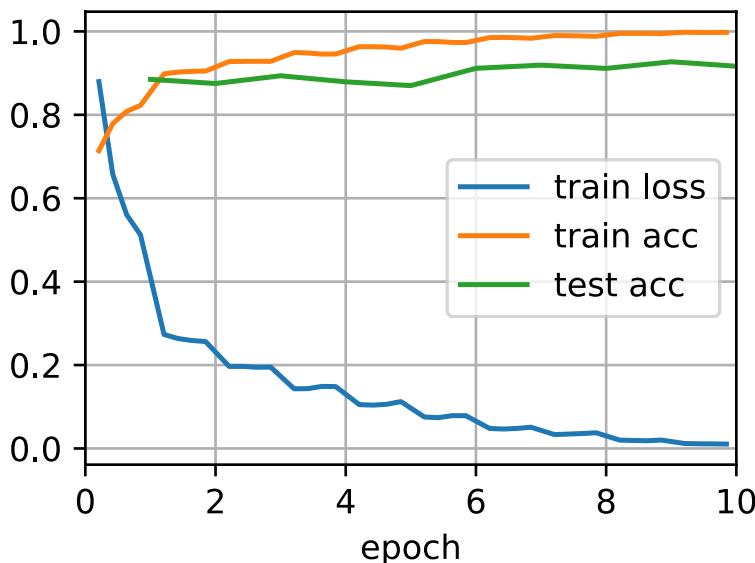
```
conv5 output shape:  (1, 64, 112, 112)
batchnorm4 output shape:      (1, 64, 112, 112)
relu0 output shape:  (1, 64, 112, 112)
pool0 output shape:  (1, 64, 56, 56)
sequential1 output shape: (1, 64, 56, 56)
sequential2 output shape: (1, 128, 28, 28)
sequential3 output shape: (1, 256, 14, 14)
sequential4 output shape: (1, 512, 7, 7)
pool1 output shape:  (1, 512, 1, 1)
dense0 output shape: (1, 10)
```

## 9.6.4 Data Acquisition and Training

We train ResNet on the Fashion-MNIST data set, just like before. The only thing that has changed is the learning rate that decreased again, due to the more complex architecture.

```
lr, num_epochs, batch_size = 0.05, 10, 256
train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size, resize=96)
d2l.train_ch5(net, train_iter, test_iter, num_epochs, lr)
```

```
loss 0.011, train acc 0.998, test acc 0.916
4726.2 examples/sec on gpu(0)
```



## 9.6.5 Summary

- Residual blocks allow for a parametrization relative to the identity function  $f(\mathbf{x}) = \mathbf{x}$ .
- Adding residual blocks increases the function complexity in a well-defined manner.
- We can train an effective deep neural network by having residual blocks pass through cross-layer data channels.

- ResNet had a major influence on the design of subsequent deep neural networks, both for convolutional and sequential nature.

### 9.6.6 Exercises

1. Refer to Table 1 in the [22] to implement different variants.
2. For deeper networks, ResNet introduces a “bottleneck” architecture to reduce model complexity. Try to implement it.
3. In subsequent versions of ResNet, the author changed the “convolution, batch normalization, and activation” architecture to the “batch normalization, activation, and convolution” architecture. Make this improvement yourself. See Figure 1 in [23] for details.
4. Prove that if  $\mathbf{x}$  is generated by a ReLU, the ResNet block does indeed include the identity function.
5. Why can't we just increase the complexity of functions without bound, even if the function classes are nested?

### 9.6.7 Scan the QR Code to Discuss<sup>126</sup>



## 9.7 Densely Connected Networks (DenseNet)

ResNet significantly changed the view of how to parametrize the functions in deep networks. DenseNet is to some extent the logical extension of this. To understand how to arrive at it, let's take a small detour to theory. Recall the Taylor expansion for functions. For scalars it can be written as

$$f(x) = f(0) + f'(x)x + \frac{1}{2}f''(x)x^2 + \frac{1}{6}f'''(x)x^3 + o(x^3) \quad (9.7.1)$$

### 9.7.1 Function Decomposition

The key point is that it decomposes the function into increasingly higher order terms. In a similar vein, ResNet decomposes functions into

$$f(\mathbf{x}) = \mathbf{x} + g(\mathbf{x}) \quad (9.7.2)$$

That is, ResNet decomposes  $f$  into a simple linear term and a more complex nonlinear one. What if we want to go beyond two terms? A solution was proposed by [26] in the form of DenseNet, an architecture that reported record performance on the ImageNet dataset.

<sup>126</sup> <https://discuss.mxnet.io/t/2359>

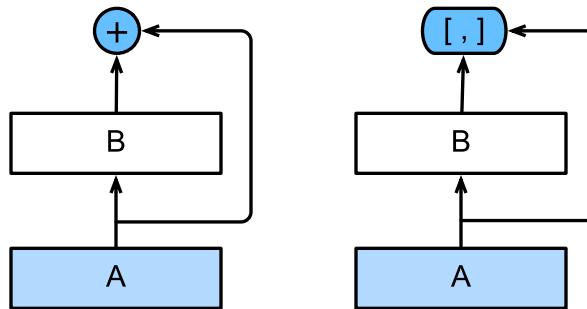


Fig. 9.7.1: The main difference between ResNet (left) and DenseNet (right) in cross-layer connections: use of addition and use of concatenation.

The key difference between ResNet and DenseNet is that in the latter case outputs are *concatenated* rather than added. As a result we perform a mapping from  $\mathbf{x}$  to its values after applying an increasingly complex sequence of functions.

$$\mathbf{x} \rightarrow [\mathbf{x}, f_1(\mathbf{x}), f_2(\mathbf{x}, f_1(\mathbf{x})), f_3(\mathbf{x}, f_1(\mathbf{x}), f_2(\mathbf{x}, f_1(\mathbf{x}))), \dots] \quad (9.7.3)$$

In the end, all these functions are combined in an MLP to reduce the number of features again. In terms of implementation this is quite simple - rather than adding terms, we concatenate them. The name DenseNet arises from the fact that the dependency graph between variables becomes quite dense. The last layer of such a chain is densely connected to all previous layers. The main components that compose a DenseNet are dense blocks and transition layers. The former defines how the inputs and outputs are concatenated, while the latter controls the number of channels so that it is not too large.

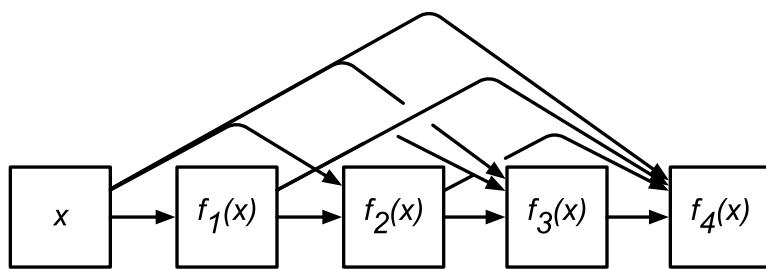


Fig. 9.7.2: Dense connections in DenseNet

## 9.7.2 Dense Blocks

DenseNet uses the modified “batch normalization, activation, and convolution” architecture of ResNet (see the exercise in Section 9.6). First, we implement this architecture in the `conv_block` function.

```
import d2l
from mxnet import gluon, nd
from mxnet.gluon import nn

def conv_block(num_channels):
    blk = nn.Sequential()
    blk.add(nn.BatchNorm(),
           nn.Activation('relu'),
```

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```
    nn.Conv2D(num_channels, kernel_size=3, padding=1))
return blk
```

A dense block consists of multiple `conv_block` units, each using the same number of output channels. In the forward computation, however, we concatenate the input and output of each block on the channel dimension.

```
class DenseBlock(nn.Block):
    def __init__(self, num_convs, num_channels, **kwargs):
        super(DenseBlock, self).__init__(**kwargs)
        self.net = nn.Sequential()
        for _ in range(num_convs):
            self.net.add(conv_block(num_channels))

    def forward(self, X):
        for blk in self.net:
            Y = blk(X)
            # Concatenate the input and output of each block on the channel
            # dimension
            X = nd.concat(X, Y, dim=1)
        return X
```

In the following example, we define a convolution block with two blocks of 10 output channels. When using an input with 3 channels, we will get an output with the  $3 + 2 \times 10 = 23$  channels. The number of convolution block channels controls the increase in the number of output channels relative to the number of input channels. This is also referred to as the growth rate.

```
blk = DenseBlock(2, 10)
blk.initialize()
X = nd.random.uniform(shape=(4, 3, 8, 8))
Y = blk(X)
Y.shape
```

```
(4, 23, 8, 8)
```

### 9.7.3 Transition Layers

Since each dense block will increase the number of channels, adding too many of them will lead to an excessively complex model. A transition layer is used to control the complexity of the model. It reduces the number of channels by using the  $1 \times 1$  convolutional layer and halves the height and width of the average pooling layer with a stride of 2, further reducing the complexity of the model.

```
def transition_block(num_channels):
    blk = nn.Sequential()
    blk.add(nn.BatchNorm(), nn.Activation('relu'),
           nn.Conv2D(num_channels, kernel_size=1),
           nn.AvgPool2D(pool_size=2, strides=2))
    return blk
```

Apply a transition layer with 10 channels to the output of the dense block in the previous example. This reduces the number of output channels to 10, and halves the height and width.

```
blk = transition_block(10)
blk.initialize()
blk(Y).shape
```

```
(4, 10, 4, 4)
```

### 9.7.4 DenseNet Model

Next, we will construct a DenseNet model. DenseNet first uses the same single convolutional layer and maximum pooling layer as ResNet.

```
net = nn.Sequential()
net.add(nn.Conv2D(64, kernel_size=7, strides=2, padding=3),
       nn.BatchNorm(), nn.Activation('relu'),
       nn.MaxPool2D(pool_size=3, strides=2, padding=1))
```

Then, similar to the four residual blocks that ResNet uses, DenseNet uses four dense blocks. Similar to ResNet, we can set the number of convolutional layers used in each dense block. Here, we set it to 4, consistent with the ResNet-18 in the previous section. Furthermore, we set the number of channels (i.e. growth rate) for the convolutional layers in the dense block to 32, so 128 channels will be added to each dense block.

In ResNet, the height and width are reduced between each module by a residual block with a stride of 2. Here, we use the transition layer to halve the height and width and halve the number of channels.

```
# Num_channels: the current number of channels
num_channels, growth_rate = 64, 32
num_convs_in_dense_blocks = [4, 4, 4, 4]

for i, num_convs in enumerate(num_convs_in_dense_blocks):
    net.add(DenseBlock(num_convs, growth_rate))
    # This is the number of output channels in the previous dense block
    num_channels += num_convs * growth_rate
    # A transition layer that halves the number of channels is added between
    # the dense blocks
    if i != len(num_convs_in_dense_blocks) - 1:
        num_channels /= 2
        net.add(transition_block(num_channels))
```

Similar to ResNet, a global pooling layer and fully connected layer are connected at the end to produce the output.

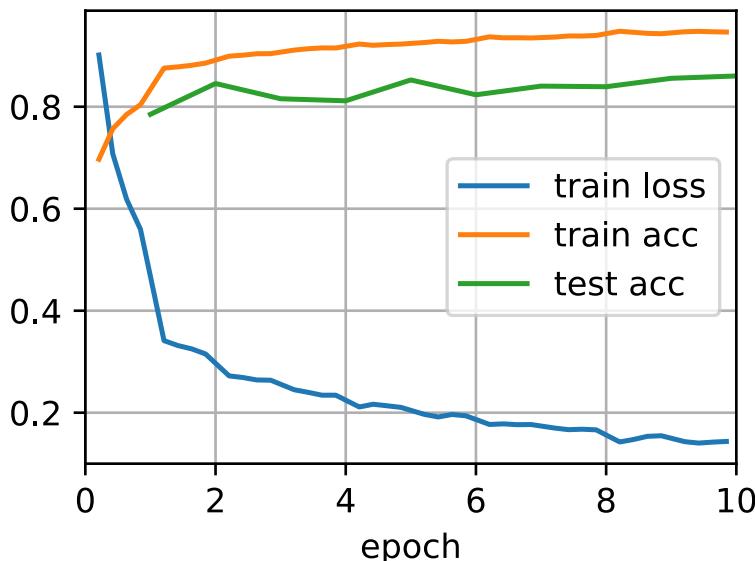
```
net.add(nn.BatchNorm(),
       nn.Activation('relu'),
       nn.GlobalAvgPool2D(),
       nn.Dense(10))
```

### 9.7.5 Data Acquisition and Training

Since we are using a deeper network here, in this section, we will reduce the input height and width from 224 to 96 to simplify the computation.

```
lr, num_epochs, batch_size = 0.1, 10, 256
train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size, resize=96)
d2l.train_ch5(net, train_iter, test_iter, num_epochs, lr)
```

```
loss 0.145, train acc 0.946, test acc 0.860
5109.2 examples/sec on gpu(0)
```



### 9.7.6 Summary

- In terms of cross-layer connections, unlike ResNet, where inputs and outputs are added together, DenseNet concatenates inputs and outputs on the channel dimension.
- The main units that compose DenseNet are dense blocks and transition layers.
- We need to keep the dimensionality under control when composing the network by adding transition layers that shrink the number of channels again.

### 9.7.7 Exercises

1. Why do we use average pooling rather than max-pooling in the transition layer?
2. One of the advantages mentioned in the DenseNet paper is that its model parameters are smaller than those of ResNet. Why is this the case?
3. One problem for which DenseNet has been criticized is its high memory consumption.
  - Is this really the case? Try to change the input shape to  $224 \times 224$  to see the actual (GPU) memory consumption.
  - Can you think of an alternative means of reducing the memory consumption? How would you need to change the framework?
4. Implement the various DenseNet versions presented in Table 1 of [26].

5. Why do we not need to concatenate terms if we are just interested in  $\mathbf{x}$  and  $f(\mathbf{x})$  for ResNet? Why do we need this for more than two layers in DenseNet?
6. Design a DenseNet for fully connected networks and apply it to the Housing Price prediction task.

#### 9.7.8 Scan the QR Code to Discuss<sup>127</sup>



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<sup>127</sup> <https://discuss.mxnet.io/t/2360>

## RECURRENT NEURAL NETWORKS

So far we encountered two types of data: generic vectors and images. For the latter we designed specialized layers to take advantage of the regularity properties in them. In other words, if we were to permute the pixels in an image, it would be much more difficult to reason about its content of something that would look much like the background of a test pattern in the times of Analog TV.

Most importantly, so far we tacitly assumed that our data is generated iid, i.e. independently and identically distributed, all drawn from some distribution. Unfortunately, this isn't true for most data. For instance, the words in this paragraph are written in sequence, and it would be quite difficult to decipher its meaning if they were permuted randomly. Likewise, image frames in a video, the audio signal in a conversation, or the browsing behavior on a website, all follow sequential order. It is thus only reasonable to assume that specialized models for such data will do better at describing it and at solving estimation problems.

Another issue arises from the fact that we might not only receive a sequence as an input but rather might be expected to continue the sequence. For instance, the task could be to continue the series 2, 4, 6, 8, 10, ... This is quite common in time series analysis, to predict the stock market, the fever curve of a patient or the acceleration needed for a race car. Again we want to have models that can handle such data.

In short, while convolutional neural networks can efficiently process spatial information, recurrent neural networks are designed to better handle sequential information. These networks introduce state variables to store past information and, together with the current input, determine the current output.

Many of the examples for using recurrent networks are based on text data. Hence, we will emphasize language models in this chapter. After a more formal review of sequence data we discuss basic concepts of a language model and use this discussion as the inspiration for the design of recurrent neural networks. Next, we describe the gradient calculation method in recurrent neural networks to explore problems that may be encountered in recurrent neural network training. For some of these problems, we can use gated recurrent neural networks, such as LSTMs (Section 10.9) and GRUs (Section 10.8), described later in this chapter.

### 10.1 Sequence Models

Imagine that you're watching movies on Netflix. As a good Netflix user you decide to rate each of the movies religiously. After all, a good movie is a good movie, and you want to watch more of them, right? As it turns out, things are not quite so simple. People's opinions on movies can change quite significantly over time. In fact, psychologists even have names for some of the effects:

- There's anchoring<sup>128</sup>, based on someone else's opinion. For instance after the Oscar awards, ratings for the corresponding movie go up, even though it's still the same movie. This effect persists for a few months until the award is forgotten. [66] showed that the effect lifts rating by over half a point.

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<sup>128</sup> <https://en.wikipedia.org/wiki/Anchoring>

- There's the Hedonic adaptation<sup>129</sup>, where humans quickly adapt to accept an improved (or a bad) situation as the new normal. For instance, after watching many good movies, the expectations that the next movie be equally good or better are high, and even an average movie might be considered a bad movie after many great ones.
- There's seasonality. Very few viewers like to watch a Santa Claus movie in August.
- In some cases movies become unpopular due to the misbehaviors of directors or actors in the production.
- Some movies become cult movies, because they were almost comically bad. *Plan 9 from Outer Space* and *Troll 2* achieved a high degree of notoriety for this reason.

In short, ratings are anything but stationary. Using temporal dynamics helped [32] to recommend movies more accurately. But it isn't just about movies.

- Many users have highly particular behavior when it comes to the time when they open apps. For instance, social media apps are much more popular after school with students. Stock market trading apps are more commonly used when the markets are open.
- It is much harder to predict tomorrow's stock prices than to fill in the blanks for a stock price we missed yesterday, even though both are just a matter of estimating one number. After all, hindsight is so much easier than foresight. In statistics the former is called *prediction* whereas the latter is called *filtering*.
- Music, speech, text, movies, steps, etc. are all sequential in nature. If we were to permute them they would make little sense. The headline *dog bites man* is much less surprising than *man bites dog*, even though the words are identical.
- Earthquakes are strongly correlated, i.e. after a massive earthquake there are very likely several smaller aftershocks, much more so than without the strong quake. In fact, earthquakes are spatiotemporally correlated, i.e. the aftershocks typically occur within a short time span and in close proximity.
- Humans interact with each other in a sequential nature, as can be seen in Twitter fights, dance patterns and debates.

### 10.1.1 Statistical Tools

In short, we need statistical tools and new deep networks architectures to deal with sequence data. To keep things simple, we use the stock price as an example.

Let's denote the prices by  $x_t \geq 0$ , i.e. at time  $t \in \mathbb{N}$  we observe some price  $x_t$ . For a trader to do well in the stock market on day  $t$  he should want to predict  $x_t$  via

$$x_t \sim p(x_t | x_{t-1}, \dots, x_1). \quad (10.1.1)$$

#### Autoregressive Models

In order to achieve this, our trader could use a regressor such as the one we trained in Section 5.3. There's just a major problem - the number of inputs,  $x_{t-1}, \dots, x_1$  varies, depending on  $t$ . That is, the number increases with the amount of data that we encounter, and we will need an approximation to make this computationally tractable. Much of what follows in this chapter will revolve around how to estimate  $p(x_t | x_{t-1}, \dots, x_1)$  efficiently. In a nutshell it boils down to two strategies:

1. Assume that the potentially rather long sequence  $x_{t-1}, \dots, x_1$  isn't really necessary. In this case we might content ourselves with some timespan  $\tau$  and only use  $x_{t-\tau}, \dots, x_{t-1}$  observations. The immediate benefit is that now the number of arguments is always the same, at least for  $t > \tau$ . This allows us

---

<sup>129</sup> [https://en.wikipedia.org/wiki/Hedonic\\_treadmill](https://en.wikipedia.org/wiki/Hedonic_treadmill)

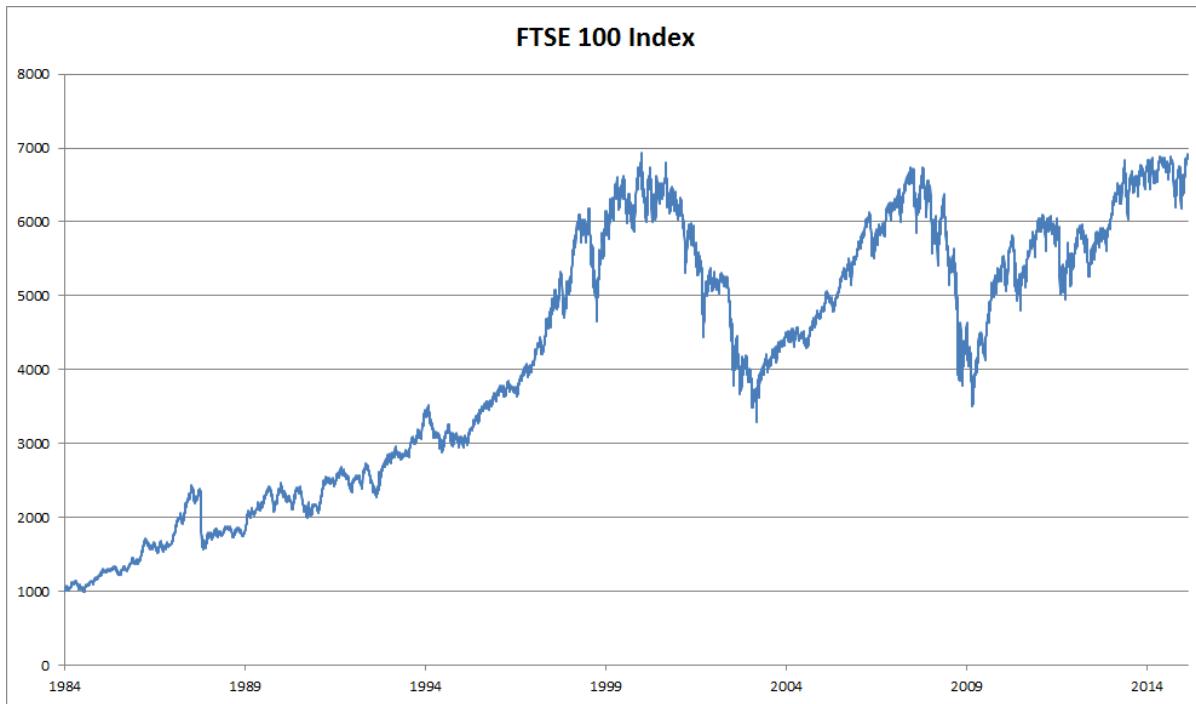


Fig. 10.1.1: FTSE 100 index over 30 years

to train a deep network as indicated above. Such models will be called *autoregressive* models, as they quite literally perform regression on themselves.

2. Another strategy is to try and keep some summary  $h_t$  of the past observations around and update that in addition to the actual prediction. This leads to models that estimate  $p(x_t|x_{t-1}, h_{t-1})$  and moreover updates of the form  $h_t = g(h_{t-1}, x_{t-1})$ . Since  $h_t$  is never observed, these models are also called *latent autoregressive models*. LSTMs and GRUs are examples of this.

Both cases raise the obvious question how to generate training data. One typically uses historical observations to predict the next observation given the ones up to right now. Obviously we do not expect time to stand still. However, a common assumption is that while the specific values of  $x_t$  might change, at least the dynamics of the time series itself won't. This is reasonable, since novel dynamics are just that, novel and thus not predictable using data we have so far. Statisticians call dynamics that don't change *stationary*. Regardless of what we do, we will thus get an estimate of the entire time series via

$$p(x_1, \dots, x_T) = \prod_{t=1}^T p(x_t|x_{t-1}, \dots, x_1). \quad (10.1.2)$$

Note that the above considerations still hold if we deal with discrete objects, such as words, rather than numbers. The only difference is that in such a situation we need to use a classifier rather than a regressor to estimate  $p(x_t|x_{t-1}, \dots, x_1)$ .

## Markov Model

Recall the approximation that in an autoregressive model we use only  $(x_{t-1}, \dots, x_{t-\tau})$  instead of  $(x_{t-1}, \dots, x_1)$  to estimate  $x_t$ . Whenever this approximation is accurate we say that the sequence satisfies a Markov

condition. In particular, if  $\tau = 1$ , we have a *first order* Markov model and  $p(x)$  is given by

$$p(x_1, \dots, x_T) = \prod_{t=1}^T p(x_t|x_{t-1}). \quad (10.1.3)$$

Such models are particularly nice whenever  $x_t$  assumes only discrete values, since in this case dynamic programming can be used to compute values along the chain exactly. For instance, we can compute  $p(x_{t+1}|x_{t-1})$  efficiently using the fact that we only need to take into account a very short history of past observations:

$$p(x_{t+1}|x_{t-1}) = \sum_{x_t} p(x_{t+1}|x_t)p(x_t|x_{t-1}). \quad (10.1.4)$$

Going into details of dynamic programming is beyond the scope of this section. Control<sup>130</sup> and reinforcement learning<sup>131</sup> algorithms use such tools extensively.

## Causality

In principle, there's nothing wrong with unfolding  $p(x_1, \dots, x_T)$  in reverse order. After all, by conditioning we can always write it via

$$p(x_1, \dots, x_T) = \prod_{t=T}^1 p(x_t|x_{t+1}, \dots, x_T). \quad (10.1.5)$$

In fact, if we have a Markov model, we can obtain a reverse conditional probability distribution, too. In many cases, however, there exists a natural direction for the data, namely going forward in time. It is clear that future events cannot influence the past. Hence, if we change  $x_t$ , we may be able to influence what happens for  $x_{t+1}$  going forward but not the converse. That is, if we change  $x_t$ , the distribution over past events will not change. Consequently, it ought to be easier to explain  $p(x_{t+1}|x_t)$  rather than  $p(x_t|x_{t+1})$ . For instance, Hoyer et al., 2008<sup>132</sup> show that in some cases we can find  $x_{t+1} = f(x_t) + \epsilon$  for some additive noise, whereas the converse is not true. This is great news, since it is typically the forward direction that we're interested in estimating. For more on this topic see e.g. the book by Peters, Janzing and Schölkopf, 2015<sup>133</sup>. We are barely scratching the surface of it.

### 10.1.2 Toy Example

After so much theory, let's try this out in practice. Since much of the modeling is identical to when we built regression estimators in Gluon, we will not delve into much detail regarding the choice of architecture besides the fact that we will use several layers of a fully connected network. Let's begin by generating some data. To keep things simple we generate our 'time series' by using a sine function with some additive noise.

```
%matplotlib inline
import d2l
from mxnet import autograd, nd, gluon, init
from mxnet.gluon import nn

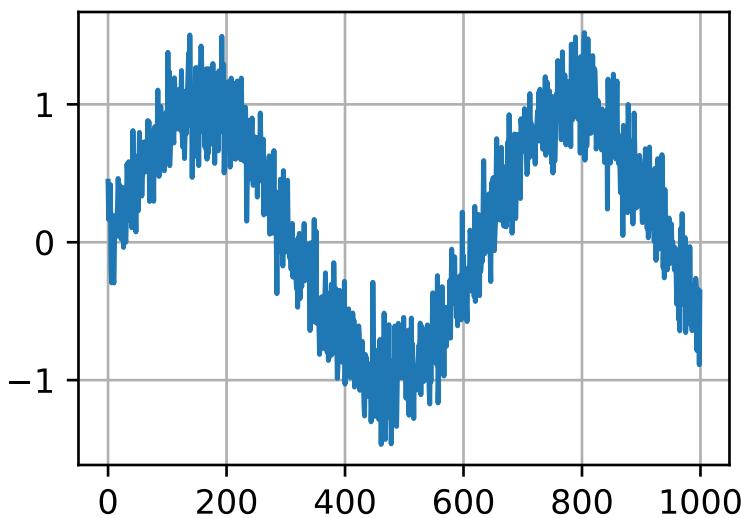
T = 1000 # Generate a total of 1000 points
time = nd.arange(0, T)
x = nd.sin(0.01 * time) + 0.2 * nd.random.normal(shape=T)
d2l.plot(time, x)
```

<sup>130</sup> [https://en.wikipedia.org/wiki/Control\\_theory](https://en.wikipedia.org/wiki/Control_theory)

<sup>131</sup> [https://en.wikipedia.org/wiki/Reinforcement\\_learning](https://en.wikipedia.org/wiki/Reinforcement_learning)

<sup>132</sup> <https://papers.nips.cc/paper/3548-nonlinear-causal-discovery-with-additive-noise-models>

<sup>133</sup> <https://mitpress.mit.edu/books/elements-causal-inference>



Next we need to turn this ‘time series’ into data the network can train on. Based on the embedding dimension  $\tau$  we map the data into pairs  $y_t = x_t$  and  $\mathbf{z}_t = (x_{t-1}, \dots, x_{t-\tau})$ . The astute reader might have noticed that this gives us  $\tau$  fewer datapoints, since we don’t have sufficient history for the first  $\tau$  of them. A simple fix, in particular if the time series is long is to discard those few terms. Alternatively we could pad the time series with zeros. The code below is essentially identical to the training code in previous sections. We kept the architecture fairly simple. A few layers of a fully connected network, ReLU activation and  $\ell_2$  loss.

```

tau = 4
features = nd.zeros((T-tau, tau))
for i in range(tau):
    features[:, i] = x[i: T-tau+i]
labels = x[tau:]

batch_size, n_train = 16, 600
train_iter = d2l.load_array((features[:n_train], labels[:n_train]),
                            batch_size, is_train=True)
test_iter = d2l.load_array((features[:n_train], labels[:n_train]),
                           batch_size, is_train=False)

# Vanilla MLP architecture
def get_net():
    net = gluon.nn.Sequential()
    net.add(nn.Dense(10, activation='relu'),
           #nn.Dense(10, activation='relu'),
           nn.Dense(1))
    net.initialize(init.Xavier())
    return net

# Least mean squares loss
loss = gluon.loss.L2Loss()

```

Now we are ready to train.

```

def train_net(net, train_iter, loss, epochs, lr):
    trainer = gluon.Trainer(net.collect_params(), 'adam',

```

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```

        {'learning_rate': lr})
for epoch in range(1, epochs + 1):
    for X, y in train_iter:
        with autograd.record():
            l = loss(net(X), y)
        l.backward()
        trainer.step(batch_size)
    print('epoch %d, loss: %f' % (
        epoch, d2l.evaluate_loss(net, train_iter, loss)))
#l = loss(net(data[:, 0]), nd.array(data[:, 1]))
#print('epoch %d, loss: %f' % (epoch, l.mean().asnumpy()))
#return net

net = get_net()
train_net(net, train_iter, loss, 10, 0.01)

#l = loss(net(test_data[:, 0]), nd.array(test_data[:, 1]))
#print('test loss: %f' % l.mean().asnumpy())

```

```

epoch 1, loss: 0.034442
epoch 2, loss: 0.029934
epoch 3, loss: 0.029162
epoch 4, loss: 0.028302
epoch 5, loss: 0.028974
epoch 6, loss: 0.027802
epoch 7, loss: 0.028245
epoch 8, loss: 0.029697
epoch 9, loss: 0.027498
epoch 10, loss: 0.028585

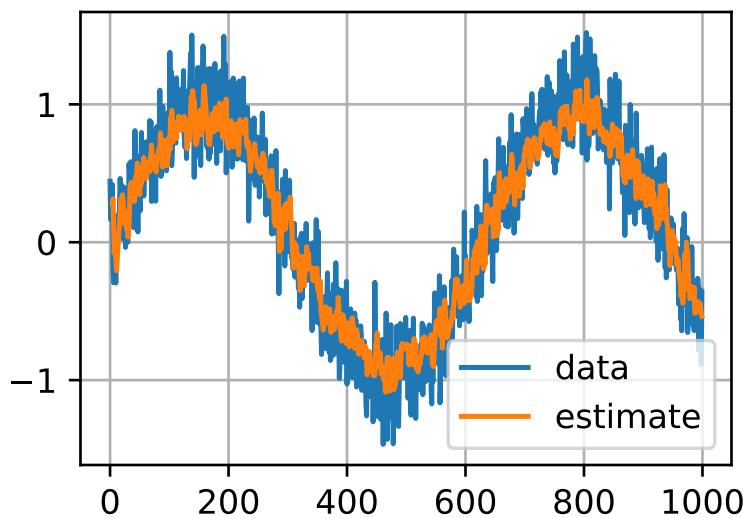
```

The both training and test loss are small and we would expect our model to work well. Let's see what this means in practice. The first thing to check is how well the model is able to predict what happens in the next timestep.

```

estimates = net(features)
d2l.plot([time, time[tau:]], [x, estimates],
         legend=['data', 'estimate'])

```



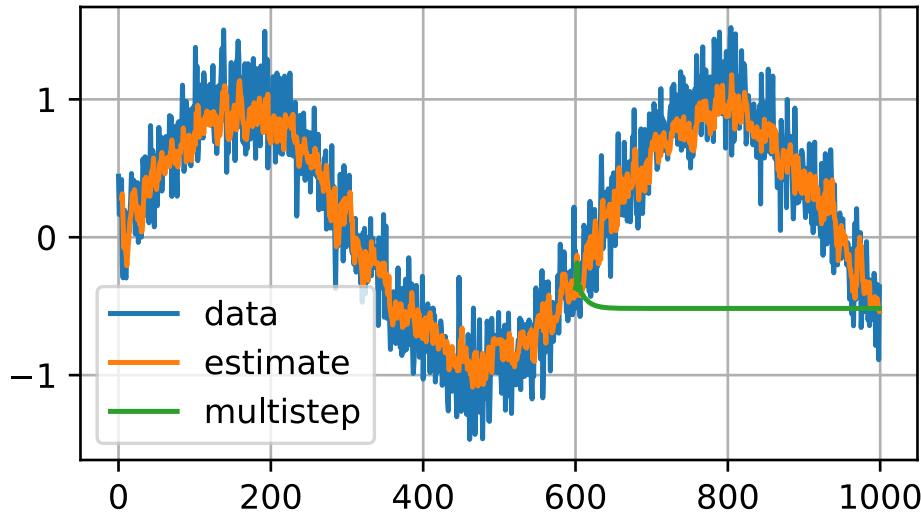
### 10.1.3 Predictions

This looks nice, just as we expected it. Even beyond 600 observations the estimates still look rather trustworthy. There's just one little problem to this - if we observe data only until time step 600, we cannot hope to receive the ground truth for all future predictions. Instead, we need to work our way forward one step at a time:

$$\begin{aligned}x_{601} &= f(x_{600}, \dots, x_{597}) \\x_{602} &= f(x_{601}, \dots, x_{598}) \\x_{603} &= f(x_{602}, \dots, x_{599})\end{aligned}\tag{10.1.6}$$

In other words, very quickly will we have to use our own predictions to make future predictions. Let's see how well this goes.

```
predictions = nd.zeros(T)
predictions[:n_train] = x[:n_train]
for i in range(n_train, T):
    predictions[i] = net(
        predictions[(i-tau):i].reshape(1,-1)).reshape(1)
d2l.plot([time, time[tau:], time[n_train:]],
         [x, estimates, predictions[n_train:]],
         legend=['data', 'estimate', 'multistep'], figsize=(4.5, 2.5))
```



As the above example shows, this is a spectacular failure. The estimates decay to a constant pretty quickly after a few prediction steps. Why did the algorithm work so poorly? This is ultimately due to the fact that errors build up. Let's say that after step 1 we have some error  $\epsilon_1 = \bar{\epsilon}$ . Now the *input* for step 2 is perturbed by  $\epsilon_1$ , hence we suffer some error in the order of  $\epsilon_2 = \bar{\epsilon} + L\epsilon_1$ , and so on. The error can diverge rather rapidly from the true observations. This is a common phenomenon - for instance weather forecasts for the next 24 hours tend to be pretty accurate but beyond that their accuracy declines rapidly. We will discuss methods for improving this throughout this chapter and beyond.

Let's verify this observation by computing the  $k$ -step predictions on the entire sequence.

```

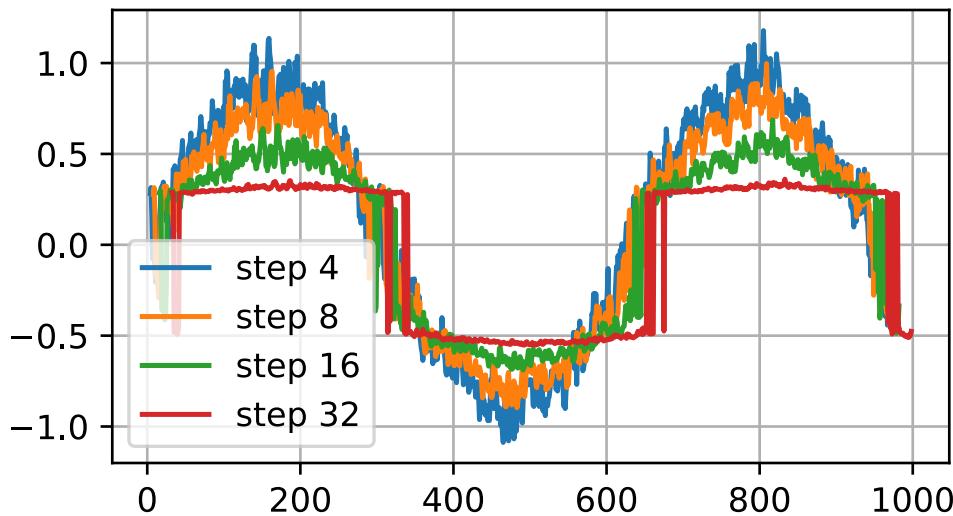
k = 33 # Look up to k - tau steps ahead

features = nd.zeros((k, T-k))
for i in range(tau): # Copy the first tau features from x
    features[i] = x[i:T-k+i]

for i in range(tau, k): # Predict the (i-tau)-th step
    features[i] = net(features[(i-tau):i].T).T

steps = (4, 8, 16, 32)
d2l.plot([time[i:T-k+i] for i in steps], [features[i] for i in steps],
         legend=['step %d'%i for i in steps], figsize=(4.5, 2.5))

```



This clearly illustrates how the quality of the estimates changes as we try to predict further into the future. While the 8-step predictions are still pretty good, anything beyond that is pretty useless.

#### 10.1.4 Summary

- Sequence models require specialized statistical tools for estimation. Two popular choices are autoregressive models and latent-variable autoregressive models.
- As we predict further in time, the errors accumulate and the quality of the estimates degrades, often dramatically.
- There's quite a difference in difficulty between filling in the blanks in a sequence (smoothing) and forecasting. Consequently, if you have a time series, always respect the temporal order of the data when training, i.e. never train on future data.
- For causal models (e.g. time going forward), estimating the forward direction is typically a lot easier than the reverse direction, i.e. we can get by with simpler networks.

#### 10.1.5 Exercises

1. Improve the above model.
  - Incorporate more than the past 4 observations? How many do you really need?
  - How many would you need if there were no noise? Hint - you can write sin and cos as a differential equation.
  - Can you incorporate older features while keeping the total number of features constant? Does this improve accuracy? Why?
  - Change the architecture and see what happens.
2. An investor wants to find a good security to buy. She looks at past returns to decide which one is likely to do well. What could possibly go wrong with this strategy?
3. Does causality also apply to text? To which extent?
4. Give an example for when a latent variable autoregressive model might be needed to capture the dynamic of the data.

### 10.1.6 Scan the QR Code to Discuss<sup>134</sup>



## 10.2 Text Preprocessing

Text is an important example of sequence data. An article can be simply viewed as a sequence of words, or a sequence of characters. Given text data is a major data format besides images we are using in this book, this section will dedicate to explain the common preprocessing steps for text data. Such preprocessing often consists of four steps:

1. Loads texts as strings into memory.
2. Splits strings into tokens, a token could be a word or a character.
3. Builds a vocabulary for these tokens to map them into numerical indices.
4. Maps all tokens in the data into indices to facilitate to feed into models.

### 10.2.1 Data Loading

To get started we load text from H. G. Wells' [Time Machine](#)<sup>135</sup>. This is a fairly small corpus of just over 30,000 words but for the purpose of what we want to illustrate this is just fine. More realistic document collections contain many billions of words. The following function read the dataset into a list of sentences, each sentence is a string. Here we ignore punctuation and capitalization.

```
import collections
import re

# Save to the d2l package.
def read_time_machine():
    """Load the time machine book into a list of sentences."""
    with open('../data/timemachine.txt', 'r') as f:
        lines = f.readlines()
    return [re.sub('[^A-Za-z]+', ' ', line.strip().lower())
            for line in lines]

lines = read_time_machine()
'# sentences %d' % len(lines)
```

```
'# sentences 3221'
```

<sup>134</sup> <https://discuss.mxnet.io/t/2860>

<sup>135</sup> <http://www.gutenberg.org/ebooks/35>

## 10.2.2 Tokenization

For each sentence, we split it into a list of tokens. A token is a data point the model will train and predict. The following function supports split a sentence into words or characters, and return a list of split sentences.

```
# Save to the d2l package.
def tokenize(lines, token='word'):
    """Split sentences into word or char tokens"""
    if token == 'word':
        return [line.split(' ') for line in lines]
    elif token == 'char':
        return [list(line) for line in lines]
    else:
        print('ERROR: unkown token type '+token)

tokens = tokenize(lines)
tokens[0:2]
```

```
[[['the', 'time', 'machine', 'by', 'h', 'g', 'wells', ''], ['']]]
```

## 10.2.3 Vocabulary

The string type of the token is inconvenient to be used by models, which take numerical inputs. Now let's build a dictionary, often called *vocabulary* as well, to map string tokens into numerical indices starting from 0. To do so, we first count the unique tokens in all documents, called *corpus*, and then assign a numerical index to each unique token according to its frequency. Rarely appeared tokens are often removed to reduce the complexity. A token doesn't exist in corpus or has been removed is mapped into a special unknown (“<unk>”) token. We optionally add another three special tokens: “<pad>” a token for padding, “<bos>” to present the beginning for a sentence, and “<eos>” for the ending of a sentence.

```
# Save to the d2l package.
class Vocab(object):
    def __init__(self, tokens, min_freq=0, use_special_tokens=False):
        # Sort according to frequencies
        counter = count_corpus(tokens)
        self.token_freqs = sorted(counter.items(), key=lambda x: x[0])
        self.token_freqs.sort(key=lambda x: x[1], reverse=True)
        if use_special_tokens:
            # padding, begin of sentence, end of sentence, unknown
            self.pad, self.bos, self.eos, self.unk = (0, 1, 2, 3)
            uniq_tokens = ['<pad>', '<bos>', '<eos>', '<unk>']
        else:
            self.unk, uniq_tokens = 0, ['<unk>']
        uniq_tokens += [token for token, freq in self.token_freqs
                        if freq >= min_freq and token not in uniq_tokens]
        self.idx_to_token, self.token_to_idx = {}, {}
        for token in uniq_tokens:
            self.idx_to_token.append(token)
            self.token_to_idx[token] = len(self.idx_to_token) - 1

    def __len__(self):
        return len(self.idx_to_token)
```

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```

def __getitem__(self, tokens):
    if not isinstance(tokens, (list, tuple)):
        return self.token_to_idx.get(tokens, self.unk)
    return [self.__getitem__(token) for token in tokens]

def to_tokens(self, indices):
    if not isinstance(indices, (list, tuple)):
        return self.idx_to_token[indices]
    return [self.idx_to_token[index] for index in indices]

# Save to the d2l package.
def count_corpus(sentences):
    # Flatten a list of token lists into a list of tokens
    tokens = [tk for line in sentences for tk in line]
    return collections.Counter(tokens)

```

We construct a vocabulary with the time machine dataset as the corpus, and then print the map between a few tokens to indices.

```

vocab = Vocab(tokens)
print(list(vocab.token_to_idx.items())[0:10])

```

```

[('<unk>', 0), ('the', 1), (' ', 2), ('i', 3), ('and', 4), ('of', 5), ('a', 6), ('to', 7),
 ← ('was', 8), ('in', 9)]

```

After that, we can convert each sentence into a list of numerical indices. To illustrate things we print two sentences with their corresponding indices.

```

for i in range(8, 10):
    print('words:', tokens[i])
    print('indices:', vocab[tokens[i]])

```

```

words: ['the', 'time', 'traveller', 'for', 'so', 'it', 'will', 'be', 'convenient', 'to',
← 'speak', 'of', 'him', '']
indices: [1, 20, 72, 17, 38, 12, 120, 43, 706, 7, 660, 5, 112, 2]
words: ['was', 'expounding', 'a', 'recondite', 'matter', 'to', 'us', 'his', 'grey', 'eyes',
← 'shone', 'and']
indices: [8, 1654, 6, 3864, 634, 7, 131, 26, 344, 127, 484, 4]

```

#### 10.2.4 Put All Things Together

We packaged the above code in the `load_corpus_time_machine` function, which returns `corpus`, a list of token indices, and `vocab`, the vocabulary. The modification we did here is that `corpus` is a single list, not a list of token lists, since we do not the sequence information in the following models. Besides, we use character tokens to simplify the training in later sections.

```

# Save to the d2l package.
def load_corpus_time_machine(max_tokens=-1):
    lines = read_time_machine()

```

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```

tokens = tokenize(lines, 'char')
vocab = Vocab(tokens)
corpus = [vocab[tk] for line in tokens for tk in line]
if max_tokens > 0: corpus = corpus[:max_tokens]
return corpus, vocab

corpus, vocab = load_corpus_time_machine()
len(corpus), len(vocab)

```

(171489, 28)

### 10.2.5 Summary

- Documents are preprocessed by tokenizing the words or characters and mapping them into indices.

### 10.2.6 Exercises

- Tokenization is a key preprocessing step. It varies for different languages. Try to find another 3 commonly used methods to tokenize sentences.

### 10.2.7 Scan the QR Code to Discuss<sup>136</sup>



## 10.3 Language Models and Data Sets

In Section 10.2, we see how to map text data into tokens, and these tokens can be viewed as a time series of discrete observations. Assuming the tokens in a text of length  $T$  are in turn  $x_1, x_2, \dots, x_T$ , then, in the discrete time series,  $x_t (1 \leq t \leq T)$  can be considered as the output or label of time step  $t$ . Given such a sequence, the goal of a language model is to estimate the probability

$$p(x_1, x_2, \dots, x_T). \quad (10.3.1)$$

Language models are incredibly useful. For instance, an ideal language model would be able to generate natural text just on its own, simply by drawing one word at a time  $w_t \sim p(w_t | w_{t-1}, \dots, w_1)$ . Quite unlike the monkey using a typewriter, all text emerging from such a model would pass as natural language, e.g. English text. Furthermore, it would be sufficient for generating a meaningful dialog, simply by conditioning the text on previous dialog fragments. Clearly we are still very far from designing such a system, since it would need to *understand* the text rather than just generate grammatically sensible content.

<sup>136</sup> <https://discuss.mxnet.io/t/2363>

Nonetheless language models are of great service even in their limited form. For instance, the phrases ‘*to recognize speech*’ and ‘*to wreck a nice beach*’ sound very similar. This can cause ambiguity in speech recognition, ambiguity that is easily resolved through a language model which rejects the second translation as outlandish. Likewise, in a document summarization algorithm it’s worth while knowing that ‘*dog bites man*’ is much more frequent than ‘*man bites dog*’, or that ‘*let’s eat grandma*’ is a rather disturbing statement, whereas ‘*let’s eat, grandma*’ is much more benign.

### 10.3.1 Estimating a language model

The obvious question is how we should model a document, or even a sequence of words. We can take recourse to the analysis we applied to sequence models in the previous section. Let’s start by applying basic probability rules:

$$p(w_1, w_2, \dots, w_T) = \prod_{t=1}^T p(w_t | w_1, \dots, w_{t-1}). \quad (10.3.2)$$

For example, the probability of a text sequence containing four tokens consisting of words and punctuation would be given as:

$$p(\text{Statistics, is, fun, .}) = p(\text{Statistics})p(\text{is}|\text{Statistics})p(\text{fun}|\text{Statistics, is})p(\cdot|\text{Statistics, is, fun}). \quad (10.3.3)$$

In order to compute the language model, we need to calculate the probability of words and the conditional probability of a word given the previous few words, i.e. language model parameters. Here, we assume that the training data set is a large text corpus, such as all Wikipedia entries, Project Gutenberg, or all text posted online on the web. The probability of words can be calculated from the relative word frequency of a given word in the training data set.

For example,  $p(\text{Statistics})$  can be calculated as the probability of any sentence starting with the word ‘statistics’. A slightly less accurate approach would be to count all occurrences of the word ‘statistics’ and divide it by the total number of words in the corpus. This works fairly well, particularly for frequent words. Moving on, we could attempt to estimate

$$\hat{p}(\text{is}|\text{Statistics}) = \frac{n(\text{Statistics is})}{n(\text{Statistics})}. \quad (10.3.4)$$

Here  $n(w)$  and  $n(w, w')$  are the number of occurrences of singletons and pairs of words respectively. Unfortunately, estimating the probability of a word pair is somewhat more difficult, since the occurrences of ‘*Statistics is*’ are a lot less frequent. In particular, for some unusual word combinations it may be tricky to find enough occurrences to get accurate estimates. Things take a turn for the worse for 3 word combinations and beyond. There will be many plausible 3-word combinations that we likely won’t see in our dataset. Unless we provide some solution to give such word combinations nonzero weight we will not be able to use these as a language model. If the dataset is small or if the words are very rare, we might not find even a single one of them.

A common strategy is to perform some form of Laplace smoothing. We already encountered this in our discussion of naive bayes in [Section 4.5](#) where the solution was to add a small constant to all counts. This helps with singletons, e.g. via

$$\begin{aligned} \hat{p}(w) &= \frac{n(w) + \epsilon_1/m}{n + \epsilon_1} \\ \hat{p}(w'|w) &= \frac{n(w, w') + \epsilon_2 \hat{p}(w')}{n(w) + \epsilon_2} \\ \hat{p}(w''|w', w) &= \frac{n(w, w', w'') + \epsilon_3 \hat{p}(w', w'')}{n(w, w') + \epsilon_3} \end{aligned} \quad (10.3.5)$$

Here the coefficients  $\epsilon_i > 0$  determine how much we use the estimate for a shorter sequence as a fill-in for longer ones. Moreover,  $m$  is the total number of words we encounter. The above is a rather primitive variant of what is Kneser-Ney smoothing and Bayesian Nonparametrics can accomplish. See e.g. the Sequence Memoizer of Wood et al., 2012 for more details of how to accomplish this. Unfortunately, models like this get unwieldy rather quickly: first off, we need to store all counts and secondly, this entirely ignores the meaning of the words. For instance, ‘cat’ and ‘feline’ should occur in related contexts. Deep learning based language models are well suited to take this into account. This, it is quite difficult to adjust such models to additional context. Lastly, long word sequences are almost certain to be novel, hence a model that simply counts the frequency of previously seen word sequences is bound to perform poorly there.

### 10.3.2 Markov Models and $n$ -grams

Before we discuss solutions involving deep learning we need some more terminology and concepts. Recall our discussion of Markov Models in the previous section. Let’s apply this to language modeling. A distribution over sequences satisfies the Markov property of first order if  $p(w_{t+1}|w_t, \dots, w_1) = p(w_{t+1}|w_t)$ . Higher orders correspond to longer dependencies. This leads to a number of approximations that we could apply to model a sequence:

$$\begin{aligned} p(w_1, w_2, w_3, w_4) &= p(w_1)p(w_2)p(w_3)p(w_4) \\ p(w_1, w_2, w_3, w_4) &= p(w_1)p(w_2|w_1)p(w_3|w_2)p(w_4|w_3) \\ p(w_1, w_2, w_3, w_4) &= p(w_1)p(w_2|w_1)p(w_3|w_1, w_2)p(w_4|w_2, w_3) \end{aligned} \quad (10.3.6)$$

Since they involve one, two or three terms, these are typically referred to as unigram, bigram and trigram models. In the following we will learn how to design better models.

### 10.3.3 Natural Language Statistics

Let’s see how this works on real data. We construct a vocabulary based on the time machine data similar to Section 10.2 and print the top words

```
import d2l
from mxnet import nd
import random

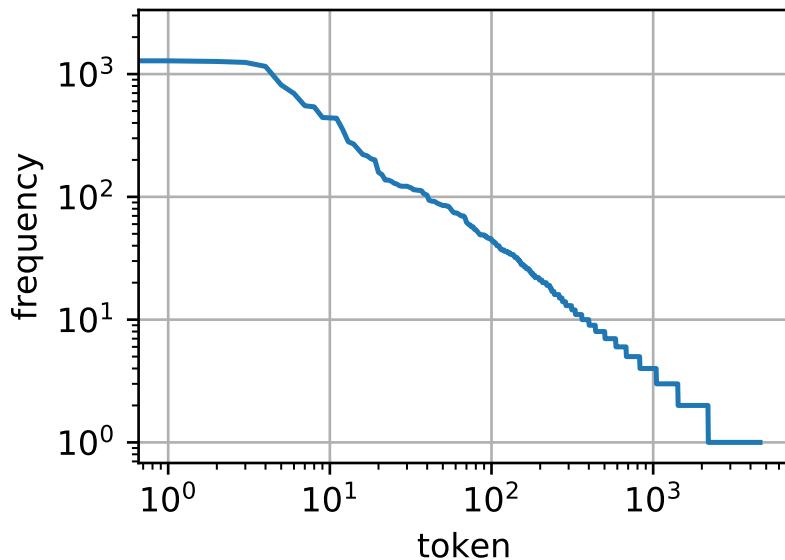
tokens = d2l.tokenize(d2l.read_time_machine())
vocab = d2l.Vocab(tokens)
print(vocab.token_freqs[:10])
```

```
[('the', 2261), ('.', 1282), ('i', 1267), ('and', 1245), ('of', 1155), ('a', 816), ('to', 695), ('was', 552), ('in', 541), ('that', 443)]
```

As we can see, the most popular words are actually quite boring to look at. They are often referred to as [stop words](#)<sup>137</sup> and thus filtered out. That said, they still carry meaning and we will use them nonetheless. However, one thing that is quite clear is that the word frequency decays rather rapidly. The 10th word is less than 1/5 as common as the most popular one. To get a better idea we plot the graph of word frequencies.

```
freqs = [freq for token, freq in vocab.token_freqs]
d2l.plot(freqs, xlabel='token', ylabel='frequency',
          xscale='log', yscale='log')
```

<sup>137</sup> [https://en.wikipedia.org/wiki/Stop\\_words](https://en.wikipedia.org/wiki/Stop_words)



We're on to something quite fundamental here - the word frequencies decay rapidly in a well defined way. After dealing with the first four words as exceptions ('the', 'i', 'and', 'of'), all remaining words follow a straight line on a log-log plot. This means that words satisfy Zipf's law<sup>138</sup> which states that the item frequency is given by

$$n(x) \propto (x + c)^{-\alpha} \text{ and hence } \log n(x) = -\alpha \log(x + c) + \text{const.} \quad (10.3.7)$$

This should already give us pause if we want to model words by count statistics and smoothing. After all, we will significantly overestimate the frequency of the tail, aka the infrequent words. But what about word pairs (and trigrams and beyond)? Let's see.

```
bigram_tokens = [[pair for pair in zip(line[:-1], line[1:])] for line in tokens]
bigram_vocab = d2l.Vocab(bigram_tokens)
print(bigram_vocab.token_freqs[:10])

[((('of', 'the'), 297), ((('in', 'the'), 161), ((('i', 'had'), 126), ((('and', 'the'), 104),
    ↪((('i', 'was'), 104), ((('the', 'time'), 97), ((('it', 'was'), 94), ((('to', 'the'), 81),
    ↪((('as', 'i'), 75), ((('of', 'a'), 69)]
```

Two things are notable. Out of the 10 most frequent word pairs, 9 are composed of stop words and only one is relevant to the actual book - 'the time'. Let's see whether the bigram frequencies behave in the same manner as the unigram frequencies.

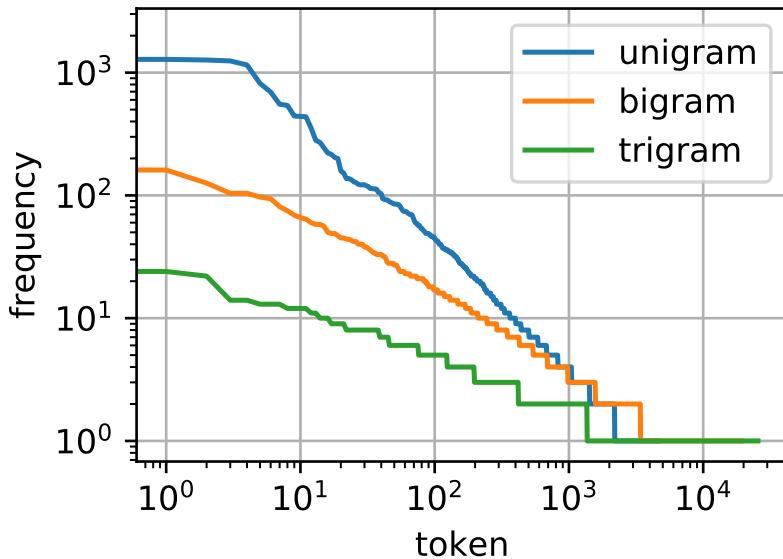
```
trigram_tokens = [[triple for triple in zip(line[:-2], line[1:-1], line[2:])] for line in tokens]
trigram_vocab = d2l.Vocab(trigram_tokens)
print(trigram_vocab.token_freqs[:10])

[((('the', 'time', 'traveller'), 53), ((('the', 'time', 'machine'), 24), ((('the', 'medical',
    ↪', 'man'), 22), ((('it', 'seemed', 'to'), 14), ((('it', 'was', 'a'), 14), ((('i', 'began',
    ↪', 'to'), 13), ((('i', 'did', 'not'), 13), ((('i', 'saw', 'the'), 13), ((('here', 'and',
    ↪', 'there'), 12), ((('i', 'could', 'see'), 12)]
```

<sup>138</sup> [https://en.wikipedia.org/wiki/Zipf%27s\\_law](https://en.wikipedia.org/wiki/Zipf%27s_law)

Last, let's visualize the token frequencies among these three gram models.

```
bigram_freqs = [freq for token, freq in bigram_vocab.token_freqs]
trigram_freqs = [freq for token, freq in trigram_vocab.token_freqs]
d2l.plot([freqs, bigram_freqs, trigram_freqs], xlabel='token',
         ylabel='frequency', xscale='log', yscale='log',
         legend=['unigram', 'bigram', 'trigram'])
```



The graph is quite exciting for a number of reasons. Firstly, beyond words, also sequences of words appear to be following Zipf's law, albeit with a lower exponent, depending on sequence length. Secondly, the number of distinct n-grams is not that large. This gives us hope that there is quite a lot of structure in language. Third, *many* n-grams occur very rarely, which makes Laplace smoothing rather unsuitable for language modeling. Instead, we will use deep learning based models.

#### 10.3.4 Training Data Preparation

Before introducing the model, let's assume we will use a neural network to train a language model. Now the question is how to read mini-batches of examples and labels at random. Since sequence data is by its very nature sequential, we need to address the issue of processing it. We did so in a rather ad-hoc manner when we introduced in [Section 10.1](#). Let's formalize this a bit.

In Fig. 10.3.1, we visualized several possible ways to obtain 5-grams in a sentence, here a token is a character. Note that we have quite some freedom since we could pick an arbitrary offset.

In fact, any one of these offsets is fine. Hence, which one should we pick? In fact, all of them are equally good. But if we pick all offsets we end up with rather redundant data due to overlap, particularly if the sequences are long. Picking just a random set of initial positions is no good either since it does not guarantee uniform coverage of the array. For instance, if we pick  $n$  elements at random out of a set of  $n$  with random replacement, the probability for a particular element not being picked is  $(1 - 1/n)^n \rightarrow e^{-1}$ . This means that we cannot expect uniform coverage this way. Even randomly permuting a set of all offsets does not offer good guarantees. Instead we can use a simple trick to get both *coverage* and *randomness*: use a random offset, after which one uses the terms sequentially. We describe how to accomplish this for both random sampling and sequential partitioning strategies below.

## The Time Machine by H. G. Wells

Fig. 10.3.1: Different offsets lead to different subsequences when splitting up text.

### Random Sampling

The following code randomly generates a minibatch from the data each time. Here, the batch size `batch_size` indicates to the number of examples in each mini-batch and `num_steps` is the length of the sequence (or time steps if we have a time series) included in each example. In random sampling, each example is a sequence arbitrarily captured on the original sequence. The positions of two adjacent random mini-batches on the original sequence are not necessarily adjacent. The target is to predict the next character based on what we've seen so far, hence the labels are the original sequence, shifted by one character.

```
# Save to the d2l package.
def seq_data_iter_random(corpus, batch_size, num_steps):
    # Offset the iterator over the data for uniform starts
    corpus = corpus[random.randint(0, num_steps):]
    # Subtract 1 extra since we need to account for label
    num_examples = ((len(corpus) - 1) // num_steps)
    example_indices = list(range(0, num_examples * num_steps, num_steps))
    random.shuffle(example_indices)
    # This returns a sequence of the length num_steps starting from pos
    data = lambda pos: corpus[pos: pos + num_steps]
    # Discard half empty batches
    num_batches = num_examples // batch_size
    for i in range(0, batch_size * num_batches, batch_size):
        # Batch_size indicates the random examples read each time
        batch_indices = example_indices[i:(i+batch_size)]
        X = [data(j) for j in batch_indices]
        Y = [data(j + 1) for j in batch_indices]
        yield nd.array(X), nd.array(Y)
```

Let us generate an artificial sequence from 0 to 30. We assume that the batch size and numbers of time steps are 2 and 5 respectively. This means that depending on the offset we can generate between 4 and 5  $(x, y)$  pairs. With a minibatch size of 2 we only get 2 minibatches.

```
my_seq = list(range(30))
for X, Y in seq_data_iter_random(my_seq, batch_size=2, num_steps=6):
    print('X: ', X, '\nY: ', Y)
```

```
X:  
[[18. 19. 20. 21. 22. 23.]  
 [ 6.  7.  8.  9. 10. 11.]]  
<NDArray 2x6 @cpu(0)>  
Y:  
[[19. 20. 21. 22. 23. 24.]  
 [ 7.  8.  9. 10. 11. 12.]]  
<NDArray 2x6 @cpu(0)>
```

### Sequential partitioning

In addition to random sampling of the original sequence, we can also make the positions of two adjacent random mini-batches adjacent in the original sequence.

```
# Save to the d2l package.  
def seq_data_iter_consecutive(corpus, batch_size, num_steps):  
    # Offset for the iterator over the data for uniform starts  
    offset = random.randint(0, num_steps)  
    # Slice out data - ignore num_steps and just wrap around  
    num_indices = ((len(corpus) - offset - 1) // batch_size) * batch_size  
    Xs = nd.array(corpus[offset:offset+num_indices])  
    Ys = nd.array(corpus[offset+1:offset+1+num_indices])  
    Xs, Ys = Xs.reshape((batch_size, -1)), Ys.reshape((batch_size, -1))  
    num_batches = Xs.shape[1] // num_steps  
    for i in range(0, num_batches * num_steps, num_steps):  
        X = Xs[:, i:(i+num_steps)]  
        Y = Ys[:, i:(i+num_steps)]  
        yield X, Y
```

Using the same settings, print input X and label Y for each mini-batch of examples read by random sampling. The positions of two adjacent random mini-batches on the original sequence are adjacent.

```
for X, Y in seq_data_iter_consecutive(my_seq, batch_size=2, num_steps=6):  
    print('X: ', X, '\nY: ', Y)
```

```
X:  
[[ 0.  1.  2.  3.  4.  5.]  
 [14. 15. 16. 17. 18. 19.]]  
<NDArray 2x6 @cpu(0)>  
Y:  
[[ 1.  2.  3.  4.  5.  6.]  
 [15. 16. 17. 18. 19. 20.]]  
<NDArray 2x6 @cpu(0)>  
X:  
[[ 6.  7.  8.  9. 10. 11.]  
 [20. 21. 22. 23. 24. 25.]]  
<NDArray 2x6 @cpu(0)>  
Y:  
[[ 7.  8.  9. 10. 11. 12.]  
 [21. 22. 23. 24. 25. 26.]]  
<NDArray 2x6 @cpu(0)>
```

Now we wrap the above two sampling functions to a class so that we can use it as a normal Gluon data iterator later.

```
# Save to the d2l package.
class SeqDataLoader(object):
    """A iterator to load sequence data"""
    def __init__(self, batch_size, num_steps, use_random_iter, max_tokens):
        if use_random_iter:
            data_iter_fn = d2l.seq_data_iter_random
        else:
            data_iter_fn = d2l.seq_data_iter_consecutive
        self.corpus, self.vocab = d2l.load_corpus_time_machine(max_tokens)
        self.get_iter = lambda: data_iter_fn(self.corpus, batch_size, num_steps)

    def __iter__(self):
        return self.get_iter()
```

Lastly, we define a function `load_data_time_machine` that returns both the data iterator and the vocabulary, so we can use it similarly as other functions with `load_data` prefix.

```
# Save to the d2l package.
def load_data_time_machine(batch_size, num_steps, use_random_iter=False,
                           max_tokens=10000):
    data_iter = SeqDataLoader(
        batch_size, num_steps, use_random_iter, max_tokens)
    return data_iter, data_iter.vocab
```

### 10.3.5 Summary

- Language models are an important technology for natural language processing.
- $n$ -grams provide a convenient model for dealing with long sequences by truncating the dependence.
- Long sequences suffer from the problem that they occur very rarely or never.
- Zipf's law governs the word distribution for both unigrams and  $n$ -grams.
- There's a lot of structure but not enough frequency to deal with infrequent word combinations efficiently via smoothing.
- The main choices for sequence partitioning are whether we pick consecutive or random sequences.
- Given the overall document length, it is usually acceptable to be slightly wasteful with the documents and discard half-empty minibatches.

### 10.3.6 Exercises

1. Suppose there are 100,000 words in the training data set. How many word frequencies and multi-word adjacent frequencies does a four-gram need to store?
2. Review the smoothed probability estimates. Why are they not accurate? Hint - we are dealing with a contiguous sequence rather than singletons.
3. How would you model a dialogue?
4. Estimate the exponent of Zipf's law for unigrams, bigrams and trigrams.

5. Which other mini-batch data sampling methods can you think of?
6. Why is it a good idea to have a random offset?
  - Does it really lead to a perfectly uniform distribution over the sequences on the document?
  - What would you have to do to make things even more uniform?
7. If we want a sequence example to be a complete sentence, what kinds of problems does this introduce in mini-batch sampling? Why would we want to do this anyway?

### 10.3.7 Scan the QR Code to Discuss<sup>139</sup>



## 10.4 Recurrent Neural Networks

In Section 10.3 we introduced  $n$ -gram models, where the conditional probability of word  $x_t$  at position  $t$  only depends on the  $n - 1$  previous words. If we want to check the possible effect of words earlier than  $t - (n - 1)$  on  $x_t$ , we need to increase  $n$ . However, the number of model parameters would also increase exponentially with it, as we need to store  $|V|^n$  numbers for a vocabulary  $V$ . Hence, rather than modeling  $p(x_t|x_{t-1}, \dots, x_{t-n+1})$  it is preferable to use a latent variable model in which we have

$$p(x_t|x_{t-1}, \dots, x_1) \approx p(x_t|x_{t-1}, h_t). \quad (10.4.1)$$

Here  $h_t$  is a *latent variable* that stores the sequence information. A latent variable is also called as *hidden variable*, *hidden state* or *hidden state variable*. The hidden state at time  $t$  could be computed based on both input  $x_{t-1}$  and hidden state  $h_{t-1}$  at time  $t - 1$ , that is

$$h_t = f(x_{t-1}, h_{t-1}). \quad (10.4.2)$$

For a sufficiently powerful function  $f$ , the latent variable model is not an approximation. After all,  $h_t$  could simply store all the data it observed so far. We discussed this in Section 10.1. But it could potentially makes both computation and storage expensive.

Note that we also use  $h$  to denote by the number of hidden units of a hidden layer. Hidden layers and hidden states refer to two very different concepts. Hidden layers are, as explained, layers that are hidden from view on the path from input to output. Hidden states are technically speaking *inputs* to whatever we do at a given step. Instead, they can only be computed by looking at data at previous iterations. In this sense they have much in common with latent variable models in statistics, such as clustering or topic models where the clusters affect the output but cannot be directly observed.

Recurrent neural networks are neural networks with hidden states. Before introducing this model, let's first revisit the multi-layer perceptron introduced in Section 6.1.

<sup>139</sup> <https://discuss.mxnet.io/t/2361>

### 10.4.1 Recurrent Networks Without Hidden States

Let's take a look at a multilayer perceptron with a single hidden layer. Given a mini-batch of instances  $\mathbf{X} \in \mathbb{R}^{n \times d}$  with sample size  $n$  and  $d$  inputs. Let the hidden layer's activation function be  $\phi$ . Hence the hidden layer's output  $\mathbf{H} \in \mathbb{R}^{n \times h}$  is calculated as

$$\mathbf{H} = \phi(\mathbf{X}\mathbf{W}_{xh} + \mathbf{b}_h). \quad (10.4.3)$$

Here, we have the weight parameter  $\mathbf{W}_{xh} \in \mathbb{R}^{d \times h}$ , bias parameter  $\mathbf{b}_h \in \mathbb{R}^{1 \times h}$ , and the number of hidden units  $h$ , for the hidden layer.

The hidden variable  $\mathbf{H}$  is used as the input of the output layer. The output layer is given by

$$\mathbf{O} = \mathbf{HW}_{hq} + \mathbf{b}_q. \quad (10.4.4)$$

Here,  $\mathbf{O} \in \mathbb{R}^{n \times q}$  is the output variable,  $\mathbf{W}_{hq} \in \mathbb{R}^{h \times q}$  is the weight parameter, and  $\mathbf{b}_q \in \mathbb{R}^{1 \times q}$  is the bias parameter of the output layer. If it is a classification problem, we can use  $\text{softmax}(\mathbf{O})$  to compute the probability distribution of the output category.

This is entirely analogous to the regression problem we solved previously in Section 10.1, hence we omit details. Suffice it to say that we can pick  $(x_t, x_{t-1})$  pairs at random and estimate the parameters  $\mathbf{W}$  and  $\mathbf{b}$  of our network via autograd and stochastic gradient descent.

### 10.4.2 Recurrent Networks with Hidden States

Matters are entirely different when we have hidden states. Let's look at the structure in some more detail. Remember that we often call iteration  $t$  as time  $t$  in an optimization algorithm, time in a recurrent neural network refers to steps within an iteration. Assume we have  $\mathbf{X}_t \in \mathbb{R}^{n \times d}$ ,  $t = 1, \dots, T$ , in an iteration. And  $\mathbf{H}_t \in \mathbb{R}^{n \times h}$  is the hidden variable of time step  $t$  from the sequence. Unlike the multilayer perceptron, here we save the hidden variable  $\mathbf{H}_{t-1}$  from the previous time step and introduce a new weight parameter  $\mathbf{W}_{hh} \in \mathbb{R}^{h \times h}$ , to describe how to use the hidden variable of the previous time step in the current time step. Specifically, the calculation of the hidden variable of the current time step is determined by the input of the current time step together with the hidden variable of the previous time step:

$$\mathbf{H}_t = \phi(\mathbf{X}_t \mathbf{W}_{xh} + \mathbf{H}_{t-1} \mathbf{W}_{hh} + \mathbf{b}_h). \quad (10.4.5)$$

Compared with (10.4.3), we added one more  $\mathbf{H}_{t-1} \mathbf{W}_{hh}$  here. From the relationship between hidden variables  $\mathbf{H}_t$  and  $\mathbf{H}_{t-1}$  of adjacent time steps, we know that those variables captured and retained the sequence's historical information up to the current time step, just like the state or memory of the neural network's current time step. Therefore, such a hidden variable is called a hidden state. Since the hidden state uses the same definition of the previous time step in the current time step, the computation of the equation above is recurrent, hence the name recurrent neural network (RNN).

There are many different RNN construction methods. RNNs with a hidden state defined by the equation above are very common. For time step  $t$ , the output of the output layer is similar to the computation in the multilayer perceptron:

$$\mathbf{O}_t = \mathbf{H}_t \mathbf{W}_{hq} + \mathbf{b}_q \quad (10.4.6)$$

RNN parameters include the weight  $\mathbf{W}_{xh} \in \mathbb{R}^{d \times h}$ ,  $\mathbf{W}_{hh} \in \mathbb{R}^{h \times h}$  of the hidden layer with the bias  $\mathbf{b}_h \in \mathbb{R}^{1 \times h}$ , and the weight  $\mathbf{W}_{hq} \in \mathbb{R}^{h \times q}$  of the output layer with the bias  $\mathbf{b}_q \in \mathbb{R}^{1 \times q}$ . It is worth mentioning that RNNs always use these model parameters, even for different time steps. Therefore, the number of RNN model parameters does not grow as the number of time steps increases.

Fig. 10.4.1 shows the computational logic of an RNN at three adjacent time steps. In time step  $t$ , the computation of the hidden state can be treated as an entry of a fully connected layer with the activation

function  $\phi$  after concatenating the input  $\mathbf{X}_t$  with the hidden state  $\mathbf{H}_{t-1}$  of the previous time step. The output of the fully connected layer is the hidden state of the current time step  $\mathbf{H}_t$ . Its model parameter is the concatenation of  $\mathbf{W}_{xh}$  and  $\mathbf{W}_{hh}$ , with a bias of  $\mathbf{b}_h$ . The hidden state of the current time step  $t$ ,  $\mathbf{H}_t$ , will participate in computing the hidden state  $\mathbf{H}_{t+1}$  of the next time step  $t + 1$ , the result of which will become the input for the fully connected output layer of the current time step.

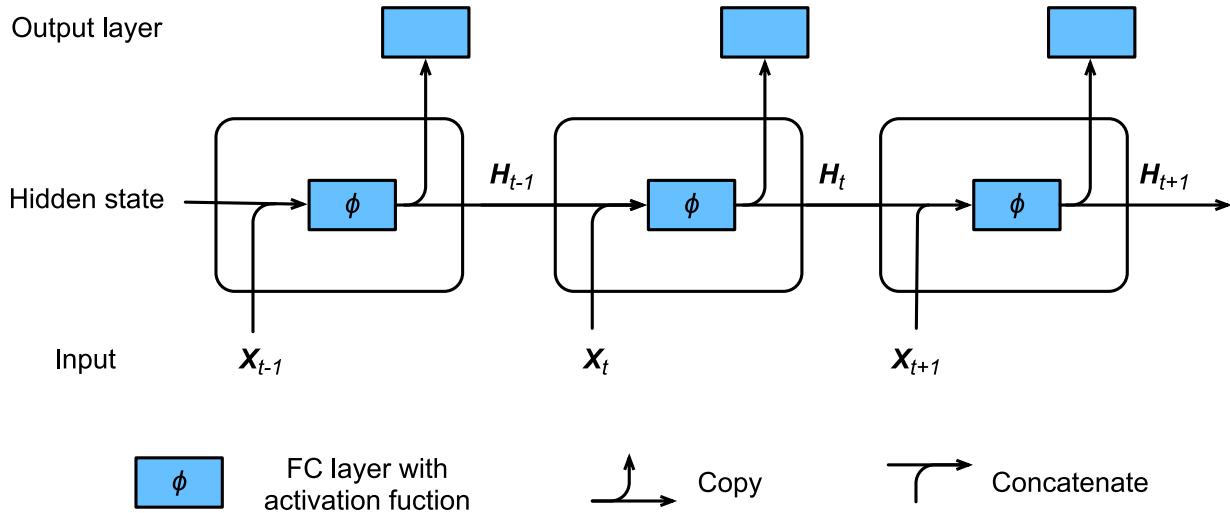


Fig. 10.4.1: An RNN with a hidden state.

### 10.4.3 Steps in a Language Model

Now we illustrate how RNNs can be used to build a language model. For simplicity of illustration we use words rather than characters, since the former are easier to comprehend. Let the number of mini-batch examples be 1, and the sequence of the text be the beginning of our dataset, i.e. “the time machine by h. g. wells”. The figure below illustrates how to estimate the next word based on the present and previous words. During the training process, we run a softmax operation on the output from the output layer for each time step, and then use the cross-entropy loss function to compute the error between the result and the label. Due to the recurrent computation of the hidden state in the hidden layer, the output of time step 3,  $\mathbf{O}_3$ , is determined by the text sequence “the”, “time”, “machine”. Since the next word of the sequence in the training data is “by”, the loss of time step 3 will depend on the probability distribution of the next word generated based on the sequence “the”, “time”, “machine” and the label “by” of this time step.

In practice, each word is presented by a  $d$  dimensional vector, and we use a batch size  $n > 1$ , therefore, the input  $\mathbf{X}_t$  at time step  $t$  will be a  $n \times d$  matrix, which is identical to what we discussed before.

### 10.4.4 Perplexity

Last, let's discuss about how to measure the sequence model quality. One way is to check how surprising the text is. A good language model is able to predict with high accuracy what we will see next. Consider the following continuations of the phrase `It is raining`, as proposed by different language models:

1. `It is raining outside`
2. `It is raining banana tree`
3. `It is raining piouw;kcj pwepoint`

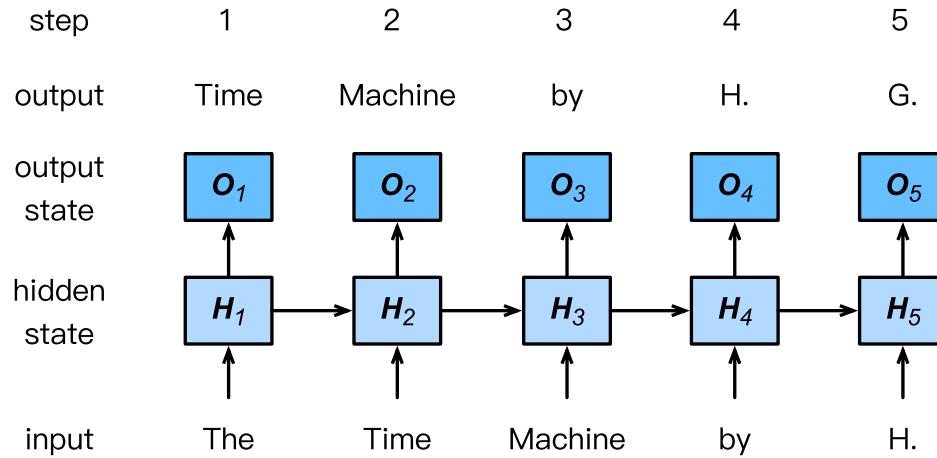


Fig. 10.4.2: Word-level RNN language model. The input and label sequences are `The Time Machine by H.` and `Time Machine by H. G.` respectively.

In terms of quality, example 1 is clearly the best. The words are sensible and logically coherent. While it might not quite so accurately reflect which word follows (`in San Francisco` and `in winter` would have been perfectly reasonable extensions), the model is able to capture which kind of word follows. Example 2 is considerably worse by producing a nonsensical and borderline dysgrammatical extension. Nonetheless, at least the model has learned how to spell words and some degree of correlation between words. Lastly, example 3 indicates a poorly trained model that doesn't fit data.

We might measure the quality of the model by computing  $p(w)$ , i.e. the likelihood of the sequence. Unfortunately this is a number that is hard to understand and difficult to compare. After all, shorter sequences are *much* more likely than long ones, hence evaluating the model on Tolstoy's magnum opus '`War and Peace`'<sup>140</sup> will inevitably produce a much smaller likelihood than, say, on Saint-Exupéry's novella '`The Little Prince`'<sup>141</sup>. What is missing is the equivalent of an average.

Information Theory comes handy here. If we want to compress text we can ask about estimating the next symbol given the current set of symbols. A lower bound on the number of bits is given by  $-\log_2 p(x_t|x_{t-1}, \dots, x_1)$ . A good language model should allow us to predict the next word quite accurately and thus it should allow us to spend very few bits on compressing the sequence. So we can measure it by the average number of bits that we need to spend.

$$\frac{1}{n} \sum_{t=1}^n -\log p(x_t|x_{t-1}, \dots, x_1) \quad (10.4.7)$$

This makes the performance on documents of different lengths comparable. For historical reasons scientists in natural language processing prefer to use a quantity called perplexity rather than bitrate. In a nutshell it is the exponential of the above:

$$\text{PPL} := \exp \left( -\frac{1}{n} \sum_{t=1}^n \log p(x_t|x_{t-1}, \dots, x_1) \right) \quad (10.4.8)$$

It can be best understood as the harmonic mean of the number of real choices that we have when deciding which word to pick next. Note that perplexity naturally generalizes the notion of the cross-entropy loss defined when we introduced the softmax regression (Section 5.4). That is, for a single symbol both definitions are identical bar the fact that one is the exponential of the other. Let's look at a number of cases:

<sup>140</sup> <https://www.gutenberg.org/files/2600/2600-h/2600-h.htm>

<sup>141</sup> [https://en.wikipedia.org/wiki/The\\_Little\\_Prince](https://en.wikipedia.org/wiki/The_Little_Prince)

- In the best case scenario, the model always estimates the probability of the next symbol as 1. In this case the perplexity of the model is 1.
- In the worst case scenario, the model always predicts the probability of the label category as 0. In this situation, the perplexity is infinite.
- At the baseline, the model predicts a uniform distribution over all tokens. In this case the perplexity equals the size of the dictionary `len(vocab)`. In fact, if we were to store the sequence without any compression this would be the best we could do to encode it. Hence this provides a nontrivial upper bound that any model must satisfy.

### 10.4.5 Summary

- A network that uses recurrent computation is called a recurrent neural network (RNN).
- The hidden state of the RNN can capture historical information of the sequence up to the current time step.
- The number of RNN model parameters does not grow as the number of time steps increases.
- We can create language models using a character-level RNN.

### 10.4.6 Exercises

1. If we use an RNN to predict the next character in a text sequence, how many output dimensions do we need?
2. Can you design a mapping for which an RNN with hidden states is exact? Hint - what about a finite number of words?
3. What happens to the gradient if you backpropagate through a long sequence?
4. What are some of the problems associated with the simple sequence model described above?

### 10.4.7 Scan the QR Code to Discuss<sup>142</sup>



## 10.5 Implementation of Recurrent Neural Networks from Scratch

In this section we implement a language model introduce in Section 10 from scratch. It is based on a character-level recurrent neural network trained on H. G. Wells' *The Time Machine*. As before, we start by reading the data set first, which is introduced in Section 10.3.

<sup>142</sup> <https://discuss.mxnet.io/t/2362>

```
%matplotlib inline
import d2l
import math
from mxnet import autograd, nd, gluon

batch_size, num_steps = 32, 35
train_iter, vocab = d2l.load_data_time_machine(batch_size, num_steps)
```

### 10.5.1 One-hot Encoding

Remember that each token is presented as a numerical index in `train_iter`. Feeding these indices directly to the neural network might make it hard to learn. We often present each token as a more expressive feature vector. The easiest presentation is called *one-hot encoding*.

In a nutshell, we map each index to a different unit vector: assume that the number of different tokens in the vocabulary is  $N$  (the `len(vocab)`) and the token indices range from 0 to  $N - 1$ . If the index of a token is the integer  $i$ , then we create a vector  $\mathbf{e}_i$  of all 0s with a length of  $N$  and set the element at position  $i$  to 1. This vector is the one-hot vector of the original token. The one-hot vectors with indices 0 and 2 are shown below.

```
nd.one_hot(nd.array([0, 2]), len(vocab))
```

```
[[1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 [0. 0. 0. 0.]]
<NDArray 2x28 @cpu(0)>
```

The shape of the mini-batch we sample each time is (batch size, time step). The `one_hot` function transforms such a mini-batch into a 3-D tensor with the last dimension equals to the vocabulary size. We often transpose the input so that we will obtain a (time step, batch size, vocabulary size) output that fits into a sequence model easier.

```
X = nd.arange(10).reshape((2, 5))
nd.one_hot(X.T, 28).shape
```

```
(5, 2, 28)
```

### 10.5.2 Initializing the Model Parameters

Next, we initialize the model parameters for a RNN model. The number of hidden units `num_hiddens` is a tunable parameter.

```
def get_params(vocab_size, num_hiddens, ctx):
    num_inputs = num_outputs = vocab_size
    normal = lambda shape: nd.random.normal(
        scale=0.01, shape=shape, ctx=ctx)
    # Hidden layer parameters
    W_xh = normal((num_inputs, num_hiddens))
    W_hh = normal((num_hiddens, num_hiddens))
```

(continues on next page)

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```
b_h = nd.zeros(num_hiddens, ctx=ctx)
# Output layer parameters
W_hq = normal((num_hiddens, num_outputs))
b_q = nd.zeros(num_outputs, ctx=ctx)
# Attach a gradient
params = [W_xh, W_hh, b_h, W_hq, b_q]
for param in params: param.attach_grad()
return params
```

### 10.5.3 RNN Model

First, we need an `init_rnn_state` function to return the hidden state at initialization. It returns a tuple consisting of an NDArray with a value of 0 and a shape of (batch size, number of hidden units). Using tuples makes it easier to handle situations where the hidden state contains multiple variables (e.g. when combining multiple layers in an RNN where each layers requires initializing).

```
def init_rnn_state(batch_size, num_hiddens, ctx):
    return (nd.zeros(shape=(batch_size, num_hiddens), ctx=ctx), )
```

The following `rnn` function defines how to compute the hidden state and output in a time step. The activation function here uses the tanh function. As described in [Section 6.1](#), the mean value of the tanh function values is 0 when the elements are evenly distributed over the real numbers.

```
def rnn(inputs, state, params):
    # inputs shape: (num_steps, batch_size, vocab_size)
    W_xh, W_hh, b_h, W_hq, b_q = params
    H, = state
    outputs = []
    for X in inputs:
        H = nd.tanh(nd.dot(X, W_xh) + nd.dot(H, W_hh) + b_h)
        Y = nd.dot(H, W_hq) + b_q
        outputs.append(Y)
    return nd.concat(*outputs, dim=0), (H,)
```

Now we have all functions defined, next we create a class to wrap these functions and store parameters.

```
# Save to the d2l package.
class RNNModelScratch(object):
    """A RNN Model based on scratch implementations"""
    def __init__(self, vocab_size, num_hiddens, ctx,
                 get_params, init_state, forward):
        self.vocab_size, self.num_hiddens = vocab_size, num_hiddens
        self.params = get_params(vocab_size, num_hiddens, ctx)
        self.init_state, self.forward_fn = init_state, forward

    def __call__(self, X, state):
        X = nd.one_hot(X.T, self.vocab_size)
        return self.forward_fn(X, state, self.params)

    def begin_state(self, batch_size, ctx):
        return self.init_state(batch_size, self.num_hiddens, ctx)
```

Let's do a sanity check whether inputs and outputs have the correct dimensions, e.g. to ensure that the dimensionality of the hidden state hasn't changed.

```
vocab_size, num_hiddens, ctx = len(vocab), 512, d2l.try_gpu()
model = RNNModelScratch(len(vocab), num_hiddens, ctx, get_params,
                        init_rnn_state, rnn)
state = model.begin_state(X.shape[0], ctx)
Y, new_state = model(X.as_in_context(ctx), state)
Y.shape, len(new_state), new_state[0].shape
```

```
((10, 28), 1, (2, 512))
```

We can see that the output shape is (number steps  $\times$  batch size, vocabulary size), while the state shape remains the same, i.e. (batch size, number of hidden units).

#### 10.5.4 Prediction

We first explain the predicting function so we can regularly check the prediction during training. This function predicts the next `num_predicts` characters based on the `prefix` (a string containing several characters). For the beginning of the sequence, we only update the hidden state. After that we begin generating new characters and emitting them.

```
# Save to the d2l package.
def predict_ch8(prefix, num_predicts, model, vocab, ctx):
    state = model.begin_state(batch_size=1, ctx=ctx)
    outputs = [vocab[prefix[0]]]
    get_input = lambda: nd.array([outputs[-1]], ctx=ctx).reshape((1, 1))
    for y in prefix[1:]: # Warmup state with prefix
        _, state = model(get_input(), state)
        outputs.append(vocab[y])
    for _ in range(num_predicts): # Predict num_predicts steps
        Y, state = model(get_input(), state)
        outputs.append(int(Y.argmax(axis=1).reshape(1).asscalar()))
    return ''.join([vocab.idx_to_token[i] for i in outputs])
```

We test the `predict_rnn` function first. Given that we didn't train the network it will generate nonsensical predictions. We initialize it with the sequence `traveller` and have it generate 10 additional characters.

```
predict_ch8('time traveller ', 10, model, vocab, ctx)
```

```
'time traveller  emmmmmmm'
```

#### 10.5.5 Gradient Clipping

For a sequence of length  $T$ , we compute the gradients over these  $T$  time steps in an iteration, which results in a chain of matrix-products with length  $O(T)$  during backpropagating. As mentioned in Section 6.8, it might result in numerical instability, e.g. the gradients may either explode or vanish, when  $T$  is large. Therefore RNN models often need extra help to stabilize the training.

Recall that when solving an optimization problem, we take update steps for the weights  $\mathbf{w}$  in the general direction of the negative gradient  $\mathbf{g}_t$  on a minibatch, say  $\mathbf{w} - \eta \cdot \mathbf{g}_t$ . Let's further assume that the objective

is well behaved, i.e. it is Lipschitz continuous with constant  $L$ , i.e.

$$|l(\mathbf{w}) - l(\mathbf{w}')| \leq L\|\mathbf{w} - \mathbf{w}'\|. \quad (10.5.1)$$

In this case we can safely assume that if we update the weight vector by  $\eta \cdot \mathbf{g}_t$  we will not observe a change by more than  $L\eta\|\mathbf{g}_t\|$ . This is both a curse and a blessing. A curse since it limits the speed with which we can make progress, a blessing since it limits the extent to which things can go wrong if we move in the wrong direction.

Sometimes the gradients can be quite large and the optimization algorithm may fail to converge. We could address this by reducing the learning rate  $\eta$  or by some other higher order trick. But what if we only rarely get large gradients? In this case such an approach may appear entirely unwarranted. One alternative is to clip the gradients by projecting them back to a ball of a given radius, say  $\theta$  via

$$\mathbf{g} \leftarrow \min\left(1, \frac{\theta}{\|\mathbf{g}\|}\right) \mathbf{g}. \quad (10.5.2)$$

By doing so we know that the gradient norm never exceeds  $\theta$  and that the updated gradient is entirely aligned with the original direction  $\mathbf{g}$ . It also has the desirable side-effect of limiting the influence any given minibatch (and within it any given sample) can exert on the weight vectors. This bestows a certain degree of robustness to the model. Gradient clipping provides a quick fix to the gradient exploding. While it doesn't entirely solve the problem, it is one of the many techniques to alleviate it.

Below we define a function to clip the gradients of a model that is either a `RNNModelScratch` instance or a Gluon model. Also note that we compute the gradient norm over all parameters.

```
# Save to the d2l package.
def grad_clipping(model, theta):
    if isinstance(model, gluon.Block):
        params = [p.data() for p in model.collect_params().values()]
    else:
        params = model.params
    norm = math.sqrt(sum((p.grad ** 2).sum() for p in params))
    if norm > theta:
        for param in params:
            param.grad[:] *= theta / norm
```

## 10.5.6 Training

Similar to Section 5.2, let's first define the function to train the model on one data epoch. It differs to the models training from previous chapters in three places:

1. Different sampling methods for sequential data (independent sampling and sequential partitioning) will result in differences in the initialization of hidden states.
2. We clip the gradient before updating the model parameters. This ensures that the model doesn't diverge even when gradients blow up at some point during the training process (effectively it reduces the stepsize automatically).
3. We use perplexity to evaluate the model. This ensures that different tests are comparable.

When the consecutive sampling is used, we initialize the hidden state at the beginning of each epoch. Since the  $i$ -th example in the next mini-batch is adjacent to the current  $i$ -th example, so the next mini-batch can use the current hidden state directly, we only detach the gradient so that we only compute the gradients within a mini-batch. When using the random sampling, we need to re-initialize the hidden state for each iteration since each example is sampled with a random position. Same to the `train_epoch_ch3` function (Section 5.2), we use generalized `updater`, which could be a Gluon trainer or a scratched implementation.

```
# Save to the d2l package.
def train_epoch_ch8(model, train_iter, loss, updater, ctx, use_random_iter):
    state, timer = None, d2l.Timer()
    metric = d2l.Accumulator(2) # loss_sum, num_examples
    for X, Y in train_iter:
        if state is None or use_random_iter:
            # Initialize state when either it's the first iteration or
            # using random sampling.
            state = model.begin_state(batch_size=X.shape[0], ctx=ctx)
        else:
            for s in state: s.detach()
        y = Y.T.reshape((-1,))
        X, y = X.as_in_context(ctx), y.as_in_context(ctx)
        with autograd.record():
            py, state = model(X, state)
            l = loss(py, y).mean()
        l.backward()
        grad_clipping(model, 1)
        updater(batch_size=1) # Since used mean already.
        metric.add(l.asscalar() * y.size, y.size)
    return math.exp(metric[0]/metric[1]), metric[1]/timer.stop()
```

The training function again supports either we implement the model from scratch or using Gluon.

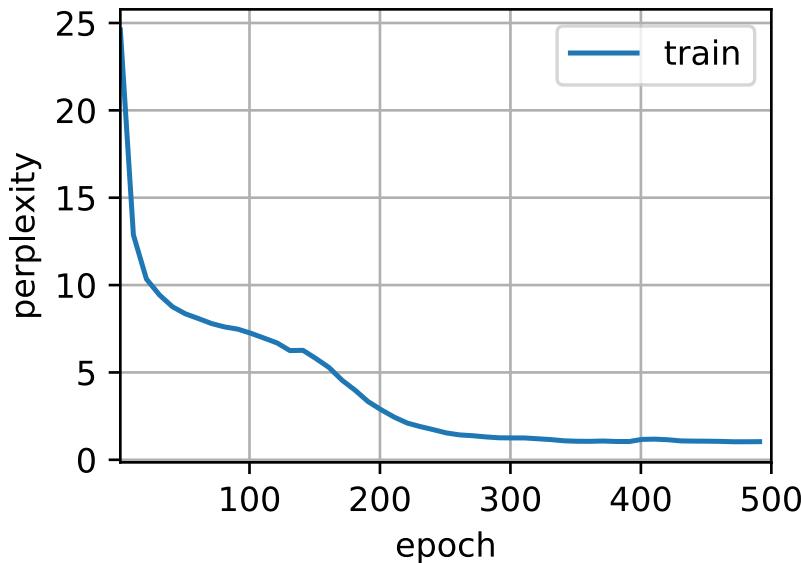
```
# Save to the d2l package.
def train_ch8(model, train_iter, vocab, lr, num_epochs, ctx,
             use_random_iter=False):
    # Initialize
    loss = gluon.loss.SoftmaxCrossEntropyLoss()
    animator = d2l.Animator(xlabel='epoch', ylabel='perplexity',
                            legend=['train'], xlim=[1, num_epochs])
    if isinstance(model, gluon.Block):
        model.initialize(ctx=ctx, force_reinit=True, init=init.Normal(0.01))
        trainer = gluon.Trainer(model.collect_params(), 'sgd', {'learning_rate': lr})
        updater = lambda batch_size : trainer.step(batch_size)
    else:
        updater = lambda batch_size : d2l.sgd(model.params, lr, batch_size)

    predict = lambda prefix: predict_ch8(prefix, 50, model, vocab, ctx)
    # Train and check the progress.
    for epoch in range(num_epochs):
        ppl, speed = train_epoch_ch8(
            model, train_iter, loss, updater, ctx, use_random_iter)
        if epoch % 10 == 0:
            print(predict('time traveller'))
            animator.add(epoch+1, [ppl])
    print('Perplexity %.1f, %d tokens/sec on %s' % (ppl, speed, ctx))
    print(predict('time traveller'))
    print(predict('traveller'))
```

Finally we can train a model. Since we only use 10,000 tokens in the dataset, so here we need more data epochs to converge.

```
num_epochs, lr = 500, 1
train_ch8(model, train_iter, vocab, lr, num_epochs, ctx)
```

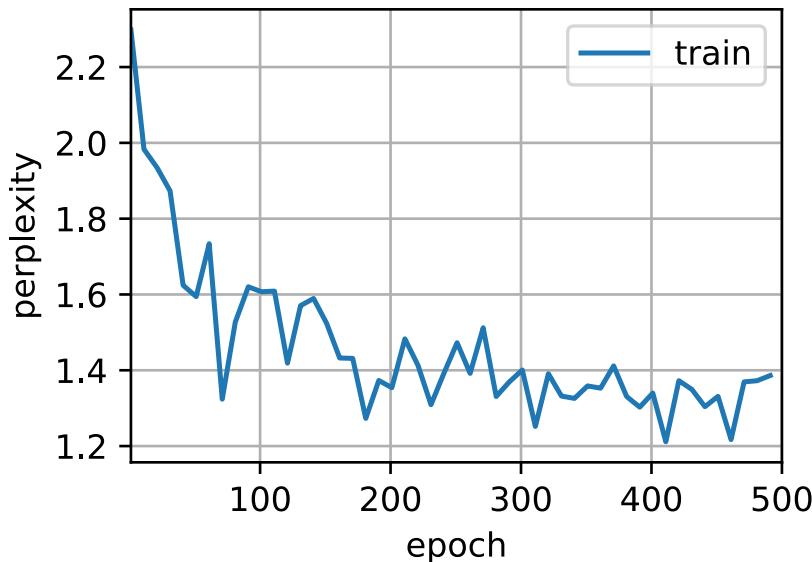
Perplexity 1.0, 42927 tokens/sec on gpu(0)  
time traveller **for** so it will be convenient to speak of him was  
traveller smiled are you sure we can move freely inspace ri



Then let's check the results to use a random sampling iterator.

```
train_ch8(model, train_iter, vocab, lr, num_epochs, ctx, use_random_iter=True)
```

Perplexity 1.3, 43963 tokens/sec on gpu(0)  
time traveller smiled **round** at us then still smiling faintly **and**  
traveller smiled **round** at us then still smiling faintly **and**



In the following we will see how to improve significantly on the current model and how to make it faster and easier to implement.

### 10.5.7 Summary

- Sequence models need state initialization for training.
- Between sequential models you need to ensure to detach the gradient, to ensure that the automatic differentiation does not propagate effects beyond the current sample.
- A simple RNN language model consists of an encoder, an RNN model and a decoder.
- Gradient clipping prevents gradient explosion (but it cannot fix vanishing gradients).
- Perplexity calibrates model performance across variable sequence length. It is the exponentiated average of the cross-entropy loss.
- Sequential partitioning typically leads to better models.

### 10.5.8 Exercises

1. Show that one-hot encoding is equivalent to picking a different embedding for each object.
2. Adjust the hyperparameters to improve the perplexity.
  - How low can you go? Adjust embeddings, hidden units, learning rate, etc.
  - How well will it work on other books by H. G. Wells, e.g. [The War of the Worlds](#)<sup>143</sup>.
3. Modify the predict function such as to use sampling rather than picking the most likely next character.
  - What happens?
  - Bias the model towards more likely outputs, e.g. by sampling from  $q(w_t|w_{t-1}, \dots, w_1) \propto p^\alpha(w_t|w_{t-1}, \dots, w_1)$  for  $\alpha > 1$ .
4. Run the code in this section without clipping the gradient. What happens?
5. Change adjacent sampling so that it does not separate hidden states from the computational graph. Does the running time change? How about the accuracy?
6. Replace the activation function used in this section with ReLU and repeat the experiments in this section.
7. Prove that the perplexity is the inverse of the harmonic mean of the conditional word probabilities.

### 10.5.9 Scan the QR Code to Discuss<sup>144</sup>



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<sup>143</sup> <http://www.gutenberg.org/ebooks/36>

<sup>144</sup> <https://discuss.mxnet.io/t/2364>

## 10.6 Concise Implementation of Recurrent Neural Networks

While Section 10.5 was instructive to see how recurrent neural networks are implemented, this isn't convenient or fast. The current section will show how to implement the same language model more efficiently using functions provided by Gluon. We begin as before by reading the 'Time Machine' corpus.

```
import d2l
import math
from mxnet import gluon, init, nd
from mxnet.gluon import nn, rnn

batch_size, num_steps = 32, 35
train_iter, vocab = d2l.load_data_time_machine(batch_size, num_steps)
```

### 10.6.1 Defining the Model

Gluon's `rnn` module provides a recurrent neural network implementation (beyond many other sequence models). We construct the recurrent neural network layer `rnn_layer` with a single hidden layer and 256 hidden units, and initialize the weights.

```
num_hiddens = 256
rnn_layer = rnn.RNN(num_hiddens)
rnn_layer.initialize()
```

Initializing the state is straightforward. We invoke the member function `rnn_layer.begin_state(batch_size)`. This returns an initial state for each element in the minibatch. That is, it returns an object that is of size (hidden layers, batch size, number of hidden units). The number of hidden layers defaults to 1. In fact, we haven't even discussed yet what it means to have multiple layers - this will happen in Section 10.10. For now, suffice it to say that multiple layers simply amount to the output of one RNN being used as the input for the next RNN.

```
batch_size = 1
state = rnn_layer.begin_state(batch_size=batch_size)
len(state), state[0].shape
```

```
(1, (1, 1, 256))
```

With a state variable and an input, we can compute the output with the updated state.

```
num_steps = 1
X = nd.random.uniform(shape=(num_steps, batch_size, len(vocab)))
Y, state_new = rnn_layer(X, state)
Y.shape, len(state_new), state_new[0].shape
```

```
((1, 1, 256), 1, (1, 1, 256))
```

Similar to Section 10.5, we define an `RNNModel` block by subclassing the `Block` class for a complete recurrent neural network. Note that `rnn_layer` only contains the hidden recurrent layers, we need to create a separate output layer. While in the previous section, we have the output layer within the `rnn` block.

```
# Save to the d2l package.
class RNNModel(nn.Block):
    def __init__(self, rnn_layer, vocab_size, **kwargs):
        super(RNNModel, self).__init__(**kwargs)
        self.rnn = rnn_layer
        self.vocab_size = vocab_size
        self.dense = nn.Dense(vocab_size)

    def forward(self, inputs, state):
        X = nd.one_hot(inputs.T, self.vocab_size)
        Y, state = self.rnn(X, state)
        # The fully connected layer will first change the shape of Y to
        # (num_steps * batch_size, num_hiddens)
        # Its output shape is (num_steps * batch_size, vocab_size)
        output = self.dense(Y.reshape((-1, Y.shape[-1])))
        return output, state

    def begin_state(self, *args, **kwargs):
        return self.rnn.begin_state(*args, **kwargs)
```

## 10.6.2 Training

Let's make a prediction with the model that has random weights.

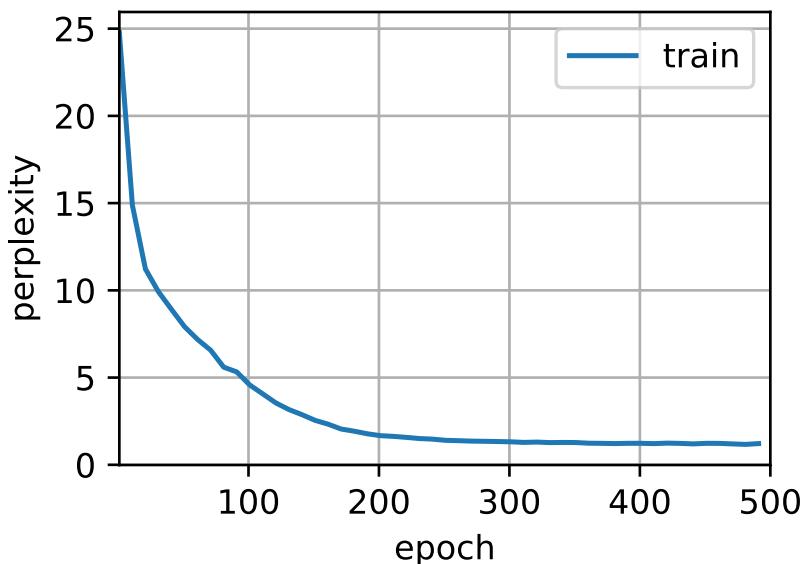
```
ctx = d2l.try_gpu()
model = RNNModel(rnn_layer, len(vocab))
model.initialize(force_reinit=True, ctx=ctx)
d2l.predict_ch8('time traveller', 10, model, vocab, ctx)
```

```
'time travellerlonu gmgmz'
```

As is quite obvious, this model doesn't work at all (just yet). Next, we call just `train_ch8` defined in Section 10.5 with the same hyper-parameters to train our model.

```
num_epochs, lr = 500, 1
d2l.train_ch8(model, train_iter, vocab, lr, num_epochs, ctx)
```

```
Perplexity 1.3, 203316 tokens/sec on gpu(0)
time traveller smiled round at us then this slips betten of spac
traveller for so ith ot ure was socting three dimensions wh
```



The model achieves comparable perplexity, albeit within a shorter period of time, due to the code being more optimized.

### 10.6.3 Summary

- Gluon's `rnn` module provides an implementation at the recurrent neural network layer.
- Gluon's `nn.RNN` instance returns the output and hidden state after forward computation. This forward computation does not involve output layer computation.
- As before, the compute graph needs to be detached from previous steps for reasons of efficiency.

### 10.6.4 Exercises

1. Compare the implementation with the previous section.
  - Why does Gluon's implementation run faster?
  - If you observe a significant difference beyond speed, try to find the reason.
2. Can you make the model overfit?
  - Increase the number of hidden units.
  - Increase the number of iterations.
  - What happens if you adjust the clipping parameter?
3. Implement the autoregressive model of the introduction to the current chapter using an RNN.
4. What happens if you increase the number of hidden layers in the RNN model? Can you make the model work?
5. How well can you compress the text using this model?
  - How many bits do you need?
  - Why doesn't everyone use this model for text compression? Hint - what about the compressor itself?

### 10.6.5 Scan the QR Code to Discuss<sup>145</sup>



## 10.7 Backpropagation Through Time

So far we repeatedly alluded to things like *exploding gradients*, *vanishing gradients*, *truncating backprop*, and the need to *detach the computational graph*. For instance, in the previous section we invoked `s.detach()` on the sequence. None of this was really fully explained, in the interest of being able to build a model quickly and to see how it works. In this section we will delve a bit more deeply into the details of backpropagation for sequence models and why (and how) the math works. For a more detailed discussion, e.g. about randomization and backprop also see the paper by Tallec and Ollivier, 2017<sup>146</sup>.

We encountered some of the effects of gradient explosion when we first implemented recurrent neural networks (Section 10.5). In particular, if you solved the problems in the problem set, you would have seen that gradient clipping is vital to ensure proper convergence. To provide a better understanding of this issue, this section will review how gradients are computed for sequences. Note that there is nothing conceptually new in how it works. After all, we are still merely applying the chain rule to compute gradients. Nonetheless it is worth while reviewing backpropagation (Section 6.7) for another time.

Forward propagation in a recurrent neural network is relatively straightforward. Back-propagation through time is actually a specific application of back propagation in recurrent neural networks. It requires us to expand the recurrent neural network one time step at a time to obtain the dependencies between model variables and parameters. Then, based on the chain rule, we apply back propagation to compute and store gradients. Since sequences can be rather long this means that the dependency can be rather lengthy. E.g. for a sequence of 1000 characters the first symbol could potentially have significant influence on the symbol at position 1000. This is not really computationally feasible (it takes too long and requires too much memory) and it requires over 1000 matrix-vector products before we would arrive at that very elusive gradient. This is a process fraught with computational and statistical uncertainty. In the following we will address what happens and how to address this in practice.

### 10.7.1 A Simplified Recurrent Network

We start with a simplified model of how an RNN works. This model ignores details about the specifics of the hidden state and how it is being updated. These details are immaterial to the analysis and would only serve to clutter the notation and make it look more intimidating.

$$h_t = f(x_t, h_{t-1}, w) \text{ and } o_t = g(h_t, w) \quad (10.7.1)$$

Here  $h_t$  denotes the hidden state,  $x_t$  the input and  $o_t$  the output. We have a chain of values  $\{\dots(h_{t-1}, x_{t-1}, o_{t-1}), (h_t, x_t, o_t), \dots\}$  that depend on each other via recursive computation. The forward pass is fairly straightforward. All we need is to loop through the  $(x_t, h_t, o_t)$  triples one step at a time. This is then evaluated by an objective function measuring the discrepancy between outputs  $o_t$  and some desired

<sup>145</sup> <https://discuss.mxnet.io/t/2365>

<sup>146</sup> <https://arxiv.org/abs/1705.08209>

target  $y_t$

$$L(x, y, w) = \sum_{t=1}^T l(y_t, o_t). \quad (10.7.2)$$

For backpropagation matters are a bit more tricky. Let's compute the gradients with regard to the parameters  $w$  of the objective function  $L$ . We get that

$$\begin{aligned} \partial_w L &= \sum_{t=1}^T \partial_w l(y_t, o_t) \\ &= \sum_{t=1}^T \partial_{o_t} l(y_t, o_t) [\partial_w g(h_t, w) + \partial_{h_t} g(h_t, w) \partial_w h_t] \end{aligned} \quad (10.7.3)$$

The first part of the derivative is easy to compute (this is after all the instantaneous loss gradient at time  $t$ ). The second part is where things get tricky, since we need to compute the effect of the parameters on  $h_t$ .

If we have three sequences  $\{a_t\}, \{b_t\}, \{c_t\}$  satisfying  $a_0 = 0, a_1 = b_1$ , and  $a_t = b_t + c_t a_{t-1}$  for  $t = 1, 2, \dots$ , then it is easy to show

$$a_t = b_t + \sum_{i=1}^{t-1} \left( \prod_{j=i+1}^t c_j \right) b_i \quad (10.7.4)$$

*for : math : 't ≥ 1', where we assume that the summation is zero when*

$t = 1$ . Therefore, the following recursion

$$\begin{aligned} \partial_w h_t &= \partial_w f(x_t, h_{t-1}, w) + \partial_h f(x_t, h_{t-1}, w) \partial_w h_{t-1} \\ &\text{implies} \end{aligned} \quad (10.7.5)$$

$$\partial_w h_t = \partial_w f(x_t, h_{t-1}, w) + \sum_{i=1}^{t-1} \left( \prod_{j=i+1}^t \partial_h f(x_j, h_{j-1}, w) \right) \partial_w f(x_i, h_{i-1}, w). \quad (10.7.6)$$

This chain can get *very* long whenever  $t$  is large. While we can use the chain rule to compute  $\partial_w h_t$  recursively, this might not be ideal. Let's discuss a number of strategies for dealing with this problem:

**Compute the full sum.** This is very slow and gradients can blow up, since subtle changes in the initial conditions can potentially affect the outcome a lot. That is, we could see things similar to the butterfly effect where minimal changes in the initial conditions lead to disproportionate changes in the outcome. This is actually quite undesirable in terms of the model that we want to estimate. After all, we are looking for robust estimators that generalize well. Hence this strategy is almost never used in practice.

**Truncate the sum after :math:`tau` steps.** This is what we've been discussing so far. This leads to an *approximation* of the true gradient, simply by terminating the sum above at  $\partial_w h_{t-\tau}$ . The approximation error is thus given by  $\partial_h f(x_t, h_{t-1}, w) \partial_w h_{t-1}$  (multiplied by a product of gradients involving  $\partial_h f$ ). In practice this works quite well. It is what is commonly referred to as truncated BPTT (backpropagation through time). One of the consequences of this is that the model focuses primarily on short-term influence rather than long-term consequences. This is actually *desirable*, since it biases the estimate towards simpler and more stable models.

**Randomized Truncation.** Lastly we can replace  $\partial_w h_t$  by a random variable which is correct in expectation but which truncates the sequence. This is achieved by using a sequence of  $\xi_t$  where  $\mathbf{E}[\xi_t] = 1$  and  $\Pr(\xi_t = 0) = 1 - \pi$  and furthermore  $\Pr(\xi_t = \pi^{-1}) = \pi$ . We use this to replace the gradient:

$$z_t = \partial_w f(x_t, h_{t-1}, w) + \xi_t \partial_h f(x_t, h_{t-1}, w) \partial_w h_{t-1} \quad (10.7.7)$$

It follows from the definition of  $\xi_t$  that  $\mathbf{E}[z_t] = \partial_w h_t$ . Whenever  $\xi_t = 0$  the expansion terminates at that point. This leads to a weighted sum of sequences of varying lengths where long sequences are rare but appropriately overweighted. Tallec and Ollivier, 2017<sup>147</sup> proposed this in their paper. Unfortunately, while appealing in theory, the model does not work much better than simple truncation, most likely due to a number of factors. Firstly, the effect of an observation after a number of backpropagation steps into the past is quite sufficient to capture dependencies in practice. Secondly, the increased variance counteracts the fact that the gradient is more accurate. Thirdly, we actually *want* models that have only a short range of interaction. Hence BPTT has a slight regularizing effect which can be desirable.

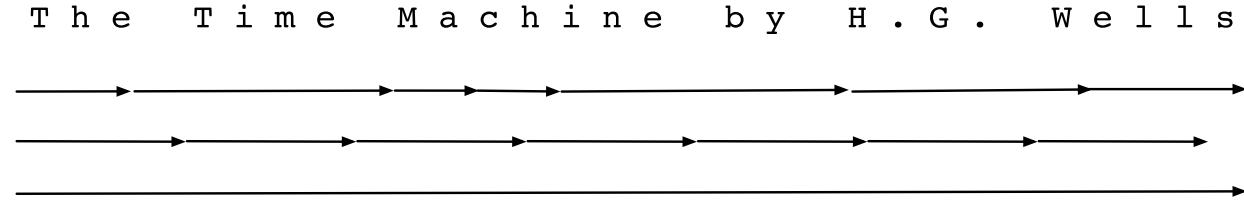


Fig. 10.7.1: From top to bottom: randomized BPTT, regularly truncated BPTT and full BPTT

The picture above illustrates the three cases when analyzing the first few words of *The Time Machine*: randomized truncation partitions the text into segments of varying length. Regular truncated BPTT breaks it into sequences of the same length, and full BPTT leads to a computationally infeasible expression.

## 10.7.2 The Computational Graph

In order to visualize the dependencies between model variables and parameters during computation in a recurrent neural network, we can draw a computational graph for the model, as shown below. For example, the computation of the hidden states of time step 3  $\mathbf{h}_3$  depends on the model parameters  $\mathbf{W}_{hx}$  and  $\mathbf{W}_{hh}$ , the hidden state of the last time step  $\mathbf{h}_2$ , and the input of the current time step  $\mathbf{x}_3$ .

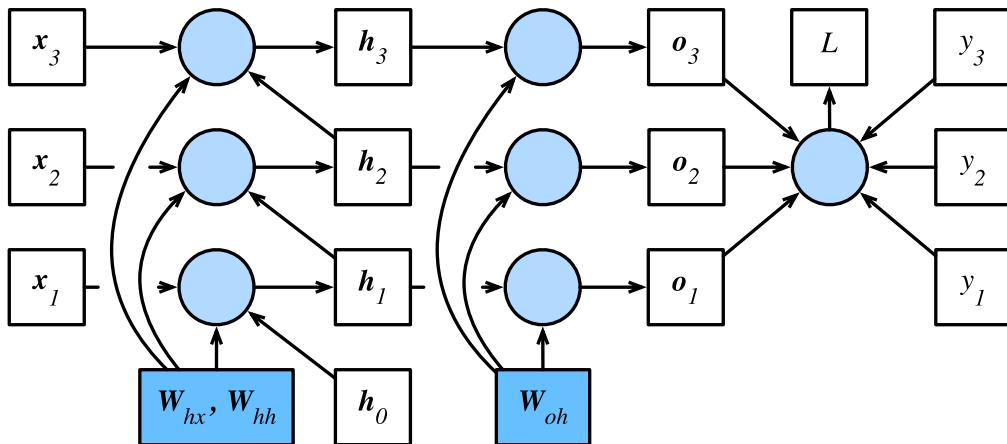


Fig. 10.7.2: Computational dependencies for a recurrent neural network model with three time steps. Boxes represent variables (not shaded) or parameters (shaded) and circles represent operators.

<sup>147</sup> <https://arxiv.org/abs/1705.08209>

### 10.7.3 BPTT in Detail

Now that we discussed the general principle let's discuss BPTT in detail, distinguishing between different sets of weight matrices ( $\mathbf{W}_{hx}$ ,  $\mathbf{W}_{hh}$  and  $\mathbf{W}_{oh}$ ) in a simple linear latent variable model:

$$\mathbf{h}_t = \mathbf{W}_{hx} \mathbf{x}_t + \mathbf{W}_{hh} \mathbf{h}_{t-1} \text{ and } \mathbf{o}_t = \mathbf{W}_{oh} \mathbf{h}_t \quad (10.7.8)$$

Following the discussion in [Section 6.7](#) we compute gradients  $\partial L / \partial \mathbf{W}_{hx}$ ,  $\partial L / \partial \mathbf{W}_{hh}$ , and  $\partial L / \partial \mathbf{W}_{oh}$  for  $L(\mathbf{x}, \mathbf{y}, \mathbf{W}) = \sum_{t=1}^T l(\mathbf{o}_t, y_t)$ . Taking the derivatives with respect to  $\mathbf{W}_{oh}$  is fairly straightforward and we obtain

$$\partial_{\mathbf{W}_{oh}} L = \sum_{t=1}^T \text{prod}(\partial_{\mathbf{o}_t} l(\mathbf{o}_t, y_t), \mathbf{h}_t) \quad (10.7.9)$$

The dependency on  $\mathbf{W}_{hx}$  and  $\mathbf{W}_{hh}$  is a bit more tricky since it involves a chain of derivatives. We begin with

$$\begin{aligned} \partial_{\mathbf{W}_{hh}} L &= \sum_{t=1}^T \text{prod}(\partial_{\mathbf{o}_t} l(\mathbf{o}_t, y_t), \mathbf{W}_{oh}, \partial_{\mathbf{W}_{hh}} \mathbf{h}_t) \\ \partial_{\mathbf{W}_{hx}} L &= \sum_{t=1}^T \text{prod}(\partial_{\mathbf{o}_t} l(\mathbf{o}_t, y_t), \mathbf{W}_{oh}, \partial_{\mathbf{W}_{hx}} \mathbf{h}_t) \end{aligned} \quad (10.7.10)$$

After all, hidden states depend on each other and on past inputs. The key quantity is how past hidden states affect future hidden states.

$$\partial_{\mathbf{h}_t} \mathbf{h}_{t+1} = \mathbf{W}_{hh}^\top \text{ and thus } \partial_{\mathbf{h}_t} \mathbf{h}_T = (\mathbf{W}_{hh}^\top)^{T-t} \quad (10.7.11)$$

Chaining terms together yields

$$\begin{aligned} \partial_{\mathbf{W}_{hh}} \mathbf{h}_t &= \sum_{j=1}^t (\mathbf{W}_{hh}^\top)^{t-j} \mathbf{h}_j \\ \partial_{\mathbf{W}_{hx}} \mathbf{h}_t &= \sum_{j=1}^t (\mathbf{W}_{hh}^\top)^{t-j} \mathbf{x}_j. \end{aligned} \quad (10.7.12)$$

A number of things follow from this potentially very intimidating expression. Firstly, it pays to store intermediate results, i.e. powers of  $\mathbf{W}_{hh}$  as we work our way through the terms of the loss function  $L$ . Secondly, this simple *linear* example already exhibits some key problems of long sequence models: it involves potentially very large powers  $\mathbf{W}_{hh}^j$ . In it, eigenvalues smaller than 1 vanish for large  $j$  and eigenvalues larger than 1 diverge. This is numerically unstable and gives undue importance to potentially irrelevant past detail. One way to address this is to truncate the sum at a computationally convenient size. Later on in this chapter we will see how more sophisticated sequence models such as LSTMs can alleviate this further. In code, this truncation is effected by *detaching* the gradient after a given number of steps.

### 10.7.4 Summary

- Back-propagation through time is merely an application of backprop to sequence models with a hidden state.
- Truncation is needed for computational convenience and numerical stability.
- High powers of matrices can lead to divergent and vanishing eigenvalues. This manifests itself in the form of exploding or vanishing gradients.
- For efficient computation intermediate values are cached.

### 10.7.5 Exercises

1. Assume that we have a symmetric matrix  $\mathbf{M} \in \mathbb{R}^{n \times n}$  with eigenvalues  $\lambda_i$ . Without loss of generality assume that they are ordered in ascending order  $\lambda_i \leq \lambda_{i+1}$ . Show that  $\mathbf{M}^k$  has eigenvalues  $\lambda_i^k$ .
2. Prove that for a random vector  $\mathbf{x} \in \mathbb{R}^n$  with high probability  $\mathbf{M}^k \mathbf{x}$  will be very much aligned with the largest eigenvector  $\mathbf{v}_n$  of  $\mathbf{M}$ . Formalize this statement.
3. What does the above result mean for gradients in a recurrent neural network?
4. Besides gradient clipping, can you think of any other methods to cope with gradient explosion in recurrent neural networks?

### 10.7.6 Scan the QR Code to Discuss<sup>148</sup>



## 10.8 Gated Recurrent Units (GRU)

In the previous section we discussed how gradients are calculated in a recurrent neural network. In particular we found that long products of matrices can lead to vanishing or divergent gradients. Let's briefly think about what such gradient anomalies mean in practice:

- We might encounter a situation where an early observation is highly significant for predicting all future observations. Consider the somewhat contrived case where the first observation contains a checksum and the goal is to discern whether the checksum is correct at the end of the sequence. In this case the influence of the first token is vital. We would like to have some mechanism for storing vital early information in a *memory cell*. Without such a mechanism we will have to assign a very large gradient to this observation, since it affects all subsequent observations.
- We might encounter situations where some symbols carry no pertinent observation. For instance, when parsing a webpage there might be auxiliary HTML code that is irrelevant for the purpose of assessing the sentiment conveyed on the page. We would like to have some mechanism for *skipping such symbols* in the latent state representation.
- We might encounter situations where there is a logical break between parts of a sequence. For instance there might be a transition between chapters in a book, a transition between a bear and a bull market for securities, etc.; In this case it would be nice to have a means of *resetting* our internal state representation.

A number of methods have been proposed to address this. One of the earliest is the Long Short Term Memory (LSTM) [24] which we will discuss in Section 10.9. The Gated Recurrent Unit (GRU) [10] is a slightly more streamlined variant that often offers comparable performance and is significantly faster to compute. See also [12] for more details. Due to its simplicity we start with the GRU.

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<sup>148</sup> <https://discuss.mxnet.io/t/2366>

### 10.8.1 Gating the Hidden State

The key distinction between regular RNNs and GRUs is that the latter support gating of the hidden state. This means that we have dedicated mechanisms for when the hidden state should be updated and also when it should be reset. These mechanisms are learned and they address the concerns listed above. For instance, if the first symbol is of great importance we will learn not to update the hidden state after the first observation. Likewise, we will learn to skip irrelevant temporary observations. Lastly, we will learn to reset the latent state whenever needed. We discuss this in detail below.

#### Reset Gates and Update Gates

The first thing we need to introduce are reset and update gates. We engineer them to be vectors with entries in  $(0, 1)$  such that we can perform convex combinations, e.g. of a hidden state and an alternative. For instance, a reset variable would allow us to control how much of the previous state we might still want to remember. Likewise, an update variable would allow us to control how much of the new state is just a copy of the old state.

We begin by engineering gates to generate these variables. The figure below illustrates the inputs for both reset and update gates in a GRU, given the current time step input  $\mathbf{X}_t$  and the hidden state of the previous time step  $\mathbf{H}_{t-1}$ . The output is given by a fully connected layer with a sigmoid as its activation function.

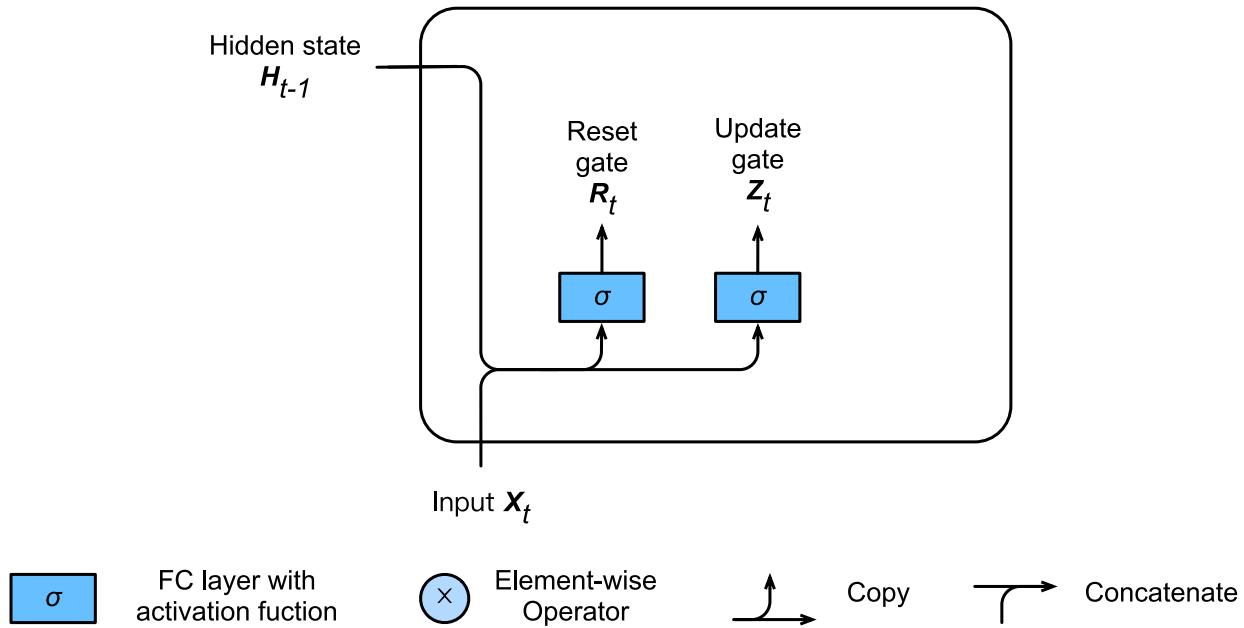


Fig. 10.8.1: Reset and update gate in a GRU.

Here, we assume there are  $h$  hidden units and, for a given time step  $t$ , the mini-batch input is  $\mathbf{X}_t \in \mathbb{R}^{n \times d}$  (number of examples:  $n$ , number of inputs:  $d$ ) and the hidden state of the last time step is  $\mathbf{H}_{t-1} \in \mathbb{R}^{n \times h}$ . Then, the reset gate  $\mathbf{R}_t \in \mathbb{R}^{n \times h}$  and update gate  $\mathbf{Z}_t \in \mathbb{R}^{n \times h}$  are computed as follows:

$$\begin{aligned}\mathbf{R}_t &= \sigma(\mathbf{X}_t \mathbf{W}_{xr} + \mathbf{H}_{t-1} \mathbf{W}_{hr} + \mathbf{b}_r) \\ \mathbf{Z}_t &= \sigma(\mathbf{X}_t \mathbf{W}_{xz} + \mathbf{H}_{t-1} \mathbf{W}_{hz} + \mathbf{b}_z)\end{aligned}\tag{10.8.1}$$

Here,  $\mathbf{W}_{xr}, \mathbf{W}_{xz} \in \mathbb{R}^{d \times h}$  and  $\mathbf{W}_{hr}, \mathbf{W}_{hz} \in \mathbb{R}^{h \times h}$  are weight parameters and  $\mathbf{b}_r, \mathbf{b}_z \in \mathbb{R}^{1 \times h}$  are biases. We use a sigmoid function (see e.g. refer to Section 6.1 for a description) to transform values to the interval  $(0, 1)$ .

### Reset Gate in Action

We begin by integrating the reset gate with a regular latent state updating mechanism. In a conventional deep RNN we would have an update of the form

$$\mathbf{H}_t = \tanh(\mathbf{X}_t \mathbf{W}_{xh} + \mathbf{H}_{t-1} \mathbf{W}_{hh} + \mathbf{b}_h). \quad (10.8.2)$$

This is essentially identical to the discussion of the previous section, albeit with a nonlinearity in the form of  $\tanh$  to ensure that the values of the hidden state remain in the interval  $(-1, 1)$ . If we want to be able to reduce the influence of previous states we can multiply  $\mathbf{H}_{t-1}$  with  $\mathbf{R}_t$  elementwise. Whenever the entries in  $\mathbf{R}_t$  are close to 1 we recover a conventional deep RNN. For all entries of  $\mathbf{R}_t$  that are close to 0 the hidden state is the result of an MLP with  $\mathbf{X}_t$  as input. Any pre-existing hidden state is thus ‘reset’ to defaults. This leads to the following candidate for a new hidden state (it is a *candidate* since we still need to incorporate the action of the update gate).

$$\tilde{\mathbf{H}}_t = \tanh(\mathbf{X}_t \mathbf{W}_{xh} + (\mathbf{R}_t \odot \mathbf{H}_{t-1}) \mathbf{W}_{hh} + \mathbf{b}_h) \quad (10.8.3)$$

The figure below illustrates the computational flow after applying the reset gate. The symbol  $\odot$  indicates pointwise multiplication between tensors.

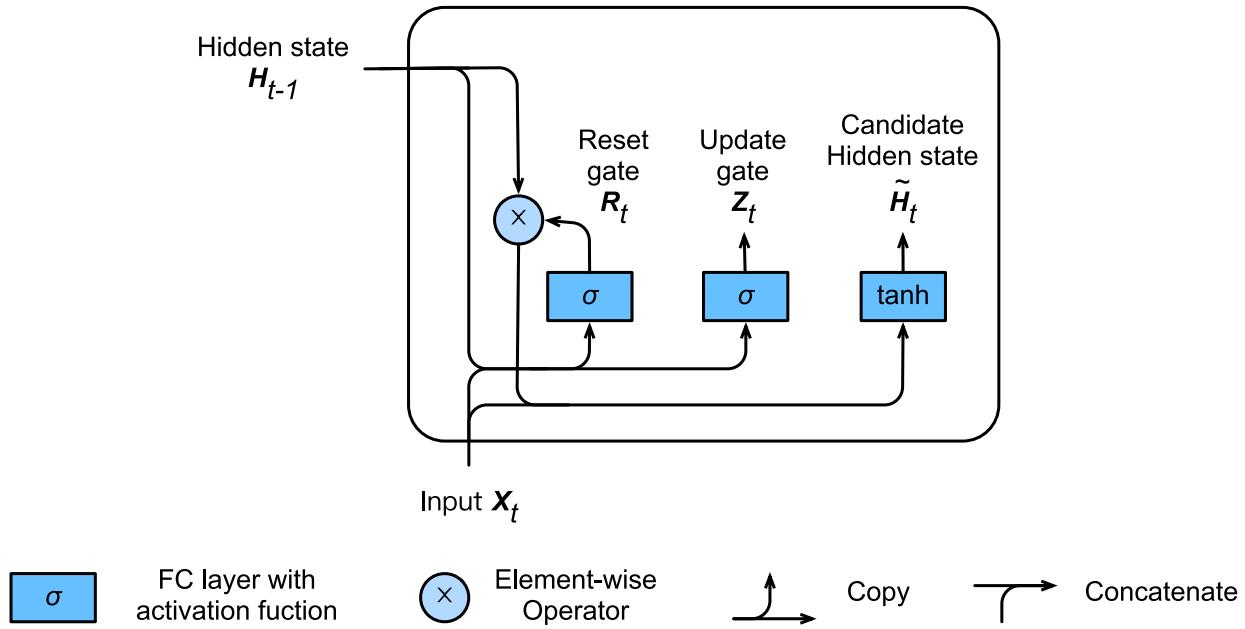


Fig. 10.8.2: Candidate hidden state computation in a GRU. The multiplication is carried out elementwise.

### Update Gate in Action

Next we need to incorporate the effect of the update gate. This determines the extent to which the new state  $\mathbf{H}_t$  is just the old state  $\mathbf{H}_{t-1}$  and by how much the new candidate state  $\tilde{\mathbf{H}}_t$  is used. The gating variable  $\mathbf{Z}_t$  can be used for this purpose, simply by taking elementwise convex combinations between both candidates. This leads to the final update equation for the GRU.

$$\mathbf{H}_t = \mathbf{Z}_t \odot \mathbf{H}_{t-1} + (1 - \mathbf{Z}_t) \odot \tilde{\mathbf{H}}_t. \quad (10.8.4)$$

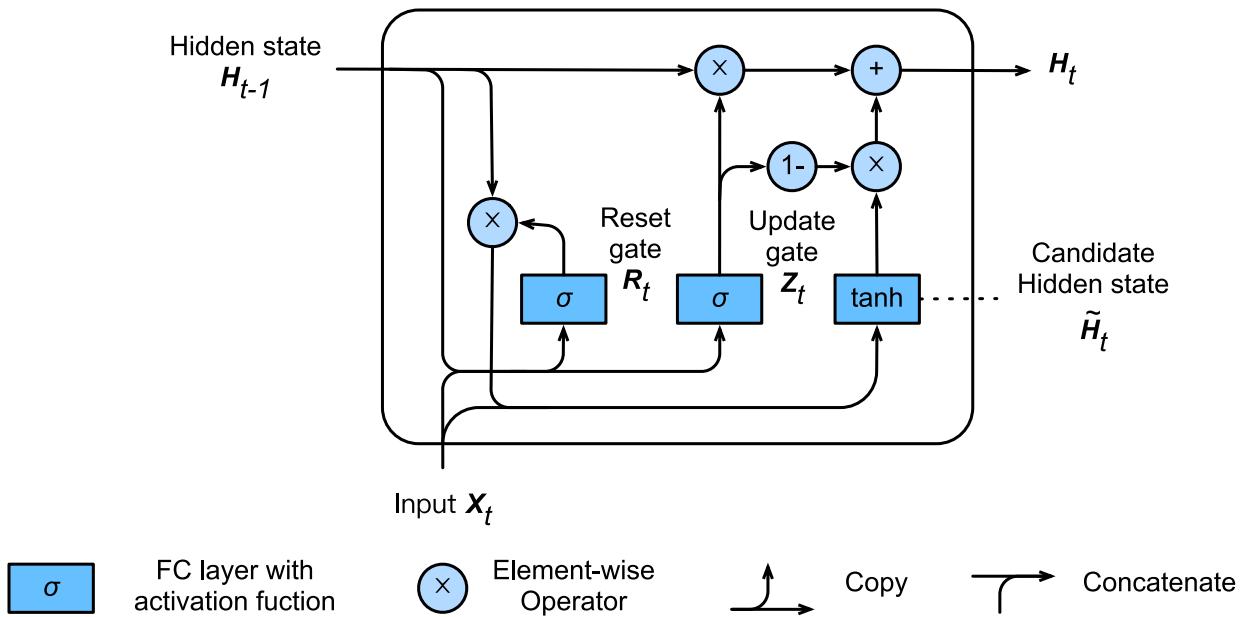


Fig. 10.8.3: Hidden state computation in a GRU. As before, the multiplication is carried out elementwise.

Whenever the update gate is close to 1 we simply retain the old state. In this case the information from  $\mathbf{X}_t$  is essentially ignored, effectively skipping time step  $t$  in the dependency chain. Whenever it is close to 1 the new latent state  $\mathbf{H}_t$  approaches the candidate latent state  $\tilde{\mathbf{H}}_t$ . These designs can help cope with the vanishing gradient problem in RNNs and better capture dependencies for time series with large time step distances. In summary GRUs have the following two distinguishing features:

- Reset gates help capture short-term dependencies in time series.
- Update gates help capture long-term dependencies in time series.

## 10.8.2 Implementation from Scratch

To gain a better understanding of the model let us implement a GRU from scratch.

### Reading the Data Set

We begin by reading *The Time Machine* corpus that we used in Section 10.5. The code for reading the data set is given below:

```
import d2l
from mxnet import nd
from mxnet.gluon import rnn

batch_size, num_steps = 32, 35
train_iter, vocab = d2l.load_data_time_machine(batch_size, num_steps)
```

## Initialize Model Parameters

The next step is to initialize the model parameters. We draw the weights from a Gaussian with variance 0.01 and set the bias to 0. The hyper-parameter `num_hiddens` defines the number of hidden units. We instantiate all terms relating to update and reset gate and the candidate hidden state itself. Subsequently we attach gradients to all parameters.

```
def get_params(vocab_size, num_hiddens, ctx):
    num_inputs = num_outputs = vocab_size
    normal = lambda shape : nd.random.normal(scale=0.01, shape=shape, ctx=ctx)
    three = lambda : (normal((num_inputs, num_hiddens)),
                      normal((num_hiddens, num_hiddens)),
                      nd.zeros(num_hiddens, ctx=ctx))
    W_xz, W_hz, b_z = three() # Update gate parameter
    W_xr, W_hr, b_r = three() # Reset gate parameter
    W_xh, W_hh, b_h = three() # Candidate hidden state parameter
    # Output layer parameters
    W_hq = normal((num_hiddens, num_outputs))
    b_q = nd.zeros(num_outputs, ctx=ctx)
    # Create gradient
    params = [W_xz, W_hz, b_z, W_xr, W_hr, b_r, W_xh, W_hh, b_h, W_hq, b_q]
    for param in params:
        param.attach_grad()
    return params
```

## Define the Model

Now we will define the hidden state initialization function `init_gru_state`. Just like the `init_rnn_state` function defined in [Section 10.5](#), this function returns a tuple composed of an NDArray with a shape (batch size, number of hidden units) and with all values set to 0.

```
def init_gru_state(batch_size, num_hiddens, ctx):
    return (nd.zeros(shape=(batch_size, num_hiddens), ctx=ctx), )
```

Now we are ready to define the actual model. Its structure is the same as the basic RNN cell, just that the update equations are more complex.

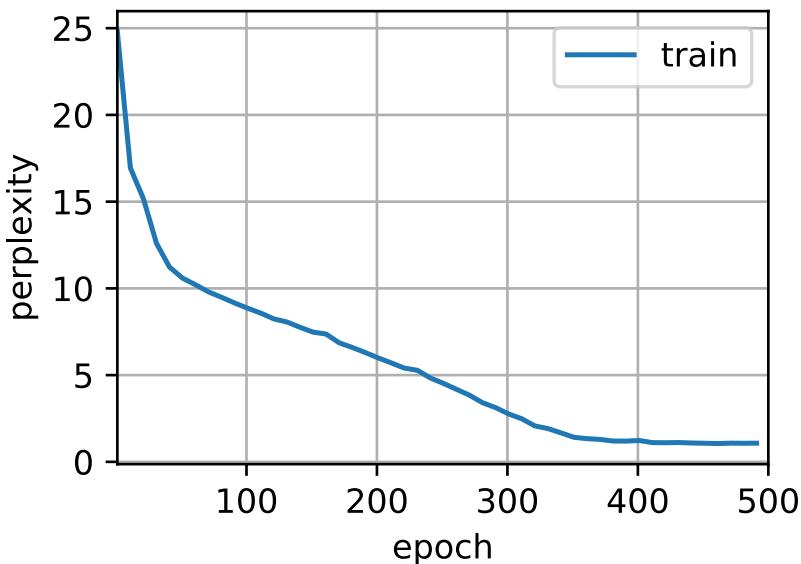
```
def gru(inputs, state, params):
    W_xz, W_hz, b_z, W_xr, W_hr, b_r, W_xh, W_hh, b_h, W_hq, b_q = params
    H, = state
    outputs = []
    for X in inputs:
        Z = nd.sigmoid(nd.dot(X, W_xz) + nd.dot(H, W_hz) + b_z)
        R = nd.sigmoid(nd.dot(X, W_xr) + nd.dot(H, W_hr) + b_r)
        H_tilda = nd.tanh(nd.dot(X, W_xh) + nd.dot(R * H, W_hh) + b_h)
        H = Z * H + (1 - Z) * H_tilda
        Y = nd.dot(H, W_hq) + b_q
        outputs.append(Y)
    return nd.concat(*outputs, dim=0), (H,)
```

## Training and Prediction

Training and prediction work in exactly the same manner as before.

```
vocab_size, num_hiddens, ctx = len(vocab), 256, d2l.try_gpu()
num_epochs, lr = 500, 1
model = d2l.RNNModelScratch(len(vocab), num_hiddens, ctx, get_params,
                             init_gru_state, gru)
d2l.train_ch8(model, train_iter, vocab, lr, num_epochs, ctx)
```

```
Perplexity 1.1, 16768 tokens/sec on gpu(0)
time traveller it's against reason said filby what reason said
traveller it's against reason said filby what reason said
```

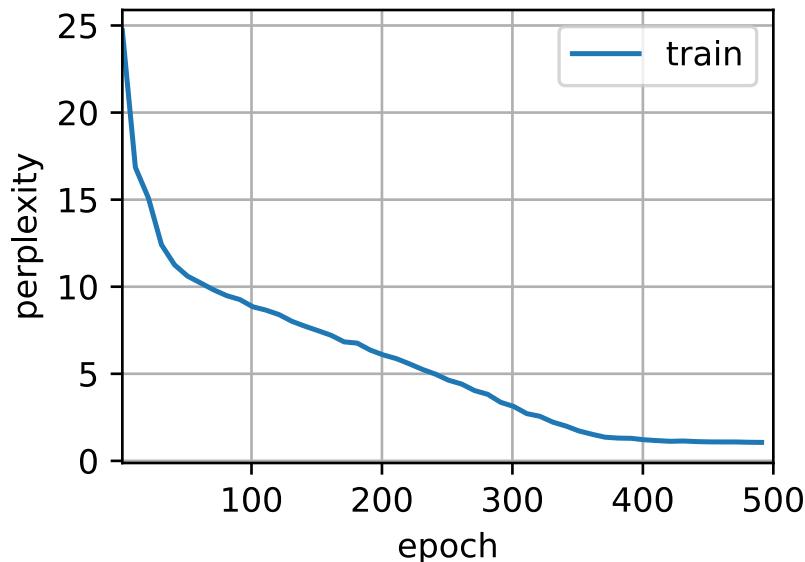


### 10.8.3 Concise Implementation

In Gluon, we can directly call the GRU class in the `rnn` module. This encapsulates all the configuration details that we made explicit above. The code is significantly faster as it uses compiled operators rather than Python for many details that we spelled out in detail before.

```
gru_layer = rnn.GRU(num_hiddens)
model = d2l.RNNModel(gru_layer, len(vocab))
d2l.train_ch8(model, train_iter, vocab, lr, num_epochs, ctx)
```

```
Perplexity 1.1, 171644 tokens/sec on gpu(0)
time traveller it's against reason said filby what reason said
traveller it's against reason said filby what reason said
```



#### 10.8.4 Summary

- Gated recurrent neural networks are better at capturing dependencies for time series with large time step distances.
- Reset gates help capture short-term dependencies in time series.
- Update gates help capture long-term dependencies in time series.
- GRUs contain basic RNNs as their extreme case whenever the reset gate is switched on. They can ignore sequences as needed.

#### 10.8.5 Exercises

1. Compare runtimes, perplexity and the extracted strings for `rnn.RNN` and `rnn.GRU` implementations with each other.
2. Assume that we only want to use the input for time step  $t'$  to predict the output at time step  $t > t'$ . What are the best values for reset and update gates for each time step?
3. Adjust the hyper-parameters and observe and analyze the impact on running time, perplexity, and the written lyrics.
4. What happens if you implement only parts of a GRU? That is, implement a recurrent cell that only has a reset gate. Likewise, implement a recurrent cell only with an update gate.

#### 10.8.6 Scan the QR Code to Discuss<sup>149</sup>

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<sup>149</sup> <https://discuss.mxnet.io/t/2367>



## 10.9 Long Short Term Memory (LSTM)

The challenge to address long-term information preservation and short-term input skipping in latent variable models has existed for a long time. One of the earliest approaches to address this was the LSTM [24]. It shares many of the properties of the Gated Recurrent Unit (GRU) and predates it by almost two decades. Its design is slightly more complex.

Arguably it is inspired by logic gates of a computer. To control a memory cell we need a number of gates. One gate is needed to read out the entries from the cell (as opposed to reading any other cell). We will refer to this as the *output* gate. A second gate is needed to decide when to read data into the cell. We refer to this as the *input* gate. Lastly, we need a mechanism to reset the contents of the cell, governed by a *forget* gate. The motivation for such a design is the same as before, namely to be able to decide when to remember and when to ignore inputs into the latent state via a dedicated mechanism. Let's see how this works in practice.

### 10.9.1 Gated Memory Cells

Three gates are introduced in LSTMs: the input gate, the forget gate, and the output gate. In addition to that we introduce memory cells that take the same shape as the hidden state. Strictly speaking this is just a fancy version of a hidden state, custom engineered to record additional information.

#### Input Gates, Forget Gates and Output Gates

Just like with GRUs, the data feeding into the LSTM gates is the input at the current time step  $\mathbf{X}_t$  and the hidden state of the previous time step  $\mathbf{H}_{t-1}$ . These inputs are processed by a fully connected layer and a sigmoid activation function to compute the values of input, forget and output gates. As a result, the three gate elements all have a value range of  $[0, 1]$ .

We assume there are  $h$  hidden units and that the minibatch is of size  $n$ . Thus the input is  $\mathbf{X}_t \in \mathbb{R}^{n \times d}$  (number of examples:  $n$ , number of inputs:  $d$ ) and the hidden state of the last time step is  $\mathbf{H}_{t-1} \in \mathbb{R}^{n \times h}$ . Correspondingly the gates are defined as follows: the input gate is  $\mathbf{I}_t \in \mathbb{R}^{n \times h}$ , the forget gate is  $\mathbf{F}_t \in \mathbb{R}^{n \times h}$ , and the output gate is  $\mathbf{O}_t \in \mathbb{R}^{n \times h}$ . They are calculated as follows:

$$\begin{aligned}\mathbf{I}_t &= \sigma(\mathbf{X}_t \mathbf{W}_{xi} + \mathbf{H}_{t-1} \mathbf{W}_{hi} + \mathbf{b}_i), \\ \mathbf{F}_t &= \sigma(\mathbf{X}_t \mathbf{W}_{xf} + \mathbf{H}_{t-1} \mathbf{W}_{hf} + \mathbf{b}_f), \\ \mathbf{O}_t &= \sigma(\mathbf{X}_t \mathbf{W}_{xo} + \mathbf{H}_{t-1} \mathbf{W}_{ho} + \mathbf{b}_o),\end{aligned}\tag{10.9.1}$$

$\mathbf{W}_{xi}, \mathbf{W}_{xf}, \mathbf{W}_{xo} \in \mathbb{R}^{d \times h}$  and  $\mathbf{W}_{hi}, \mathbf{W}_{hf}, \mathbf{W}_{ho} \in \mathbb{R}^{h \times h}$  are weight parameters and  $\mathbf{b}_i, \mathbf{b}_f, \mathbf{b}_o \in \mathbb{R}^{1 \times h}$  are bias parameters.

#### Candidate Memory Cell

Next we design a memory cell. Since we haven't specified the action of the various gates yet, we first introduce a *candidate* memory cell  $\tilde{\mathbf{C}}_t \in \mathbb{R}^{n \times h}$ . Its computation is similar to the three gates described above,

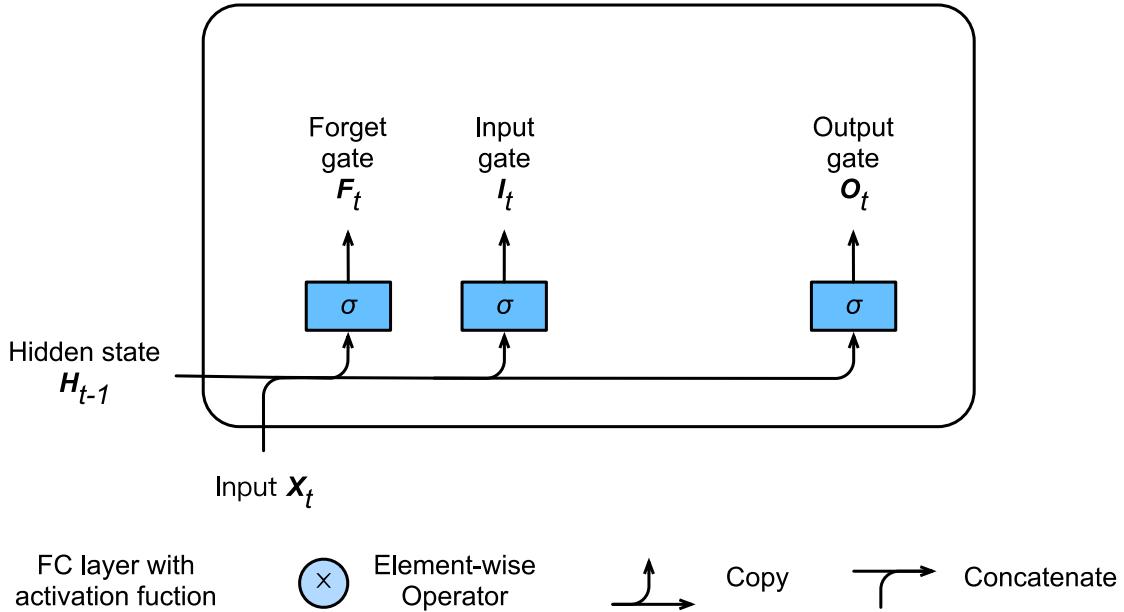


Fig. 10.9.1: Calculation of input, forget, and output gates in an LSTM.

but using a tanh function with a value range for  $[-1, 1]$  as activation function. This leads to the following equation at time step  $t$ .

$$\tilde{\mathbf{C}}_t = \tanh(\mathbf{X}_t \mathbf{W}_{xc} + \mathbf{H}_{t-1} \mathbf{W}_{hc} + \mathbf{b}_c) \quad (10.9.2)$$

Here  $\mathbf{W}_{xc} \in \mathbb{R}^{d \times h}$  and  $\mathbf{W}_{hc} \in \mathbb{R}^{h \times h}$  are weights and  $\mathbf{b}_c \in \mathbb{R}^{1 \times h}$  is a bias.

### Memory Cell

In GRUs we had a single mechanism to govern input and forgetting. Here we have two parameters,  $\mathbf{I}_t$  which governs how much we take new data into account via  $\tilde{\mathbf{C}}_t$  and the forget parameter  $\mathbf{F}_t$  which addresses how much we of the old memory cell content  $\mathbf{C}_{t-1} \in \mathbb{R}^{n \times h}$  we retain. Using the same pointwise multiplication trick as before we arrive at the following update equation.

$$\mathbf{C}_t = \mathbf{F}_t \odot \mathbf{C}_{t-1} + \mathbf{I}_t \odot \tilde{\mathbf{C}}_t. \quad (10.9.3)$$

If the forget gate is always approximately 1 and the input gate is always approximately 0, the past memory cells will be saved over time and passed to the current time step. This design was introduced to alleviate the vanishing gradient problem and to better capture dependencies for time series with long range dependencies. We thus arrive at the following flow diagram.

### Hidden States

Lastly we need to define how to compute the hidden state  $\mathbf{H}_t \in \mathbb{R}^{n \times h}$ . This is where the output gate comes into play. In the LSTM it is simply a gated version of the tanh of the memory cell. This ensures that the values of  $\mathbf{H}_t$  are always in the interval  $[-1, 1]$ . Whenever the output gate is 1 we effectively pass all memory information through to the predictor whereas for output 0 we retain all information only within the memory cell and perform no further processing. The figure below has a graphical illustration of the data flow.

$$\mathbf{H}_t = \mathbf{O}_t \odot \tanh(\mathbf{C}_t). \quad (10.9.4)$$

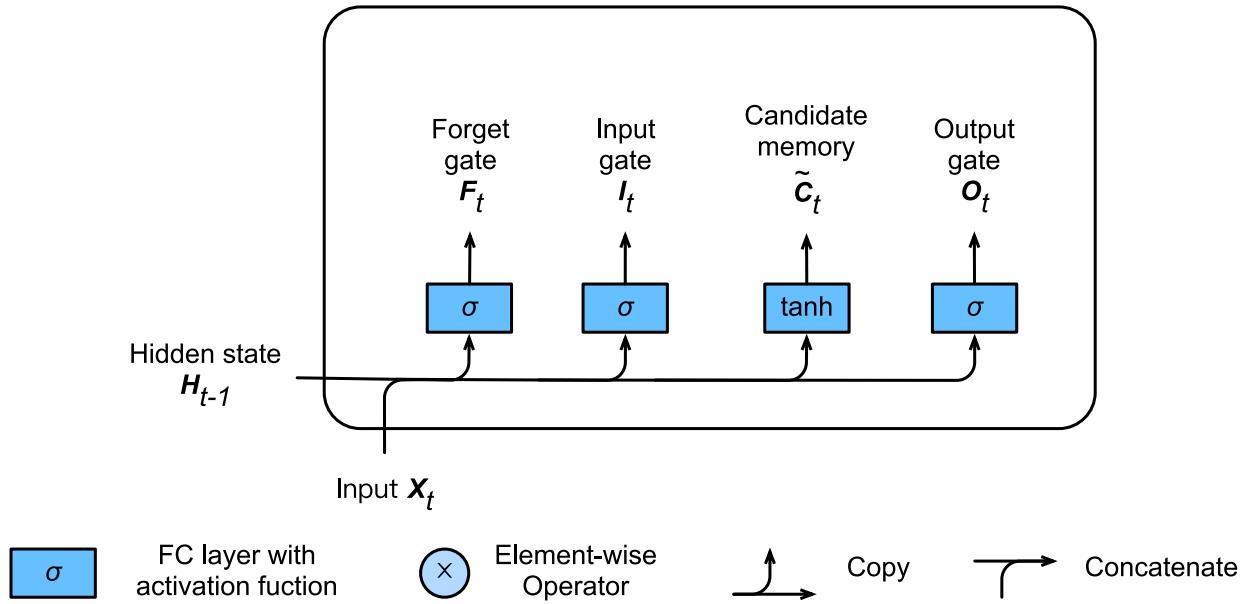


Fig. 10.9.2: Computation of candidate memory cells in LSTM.

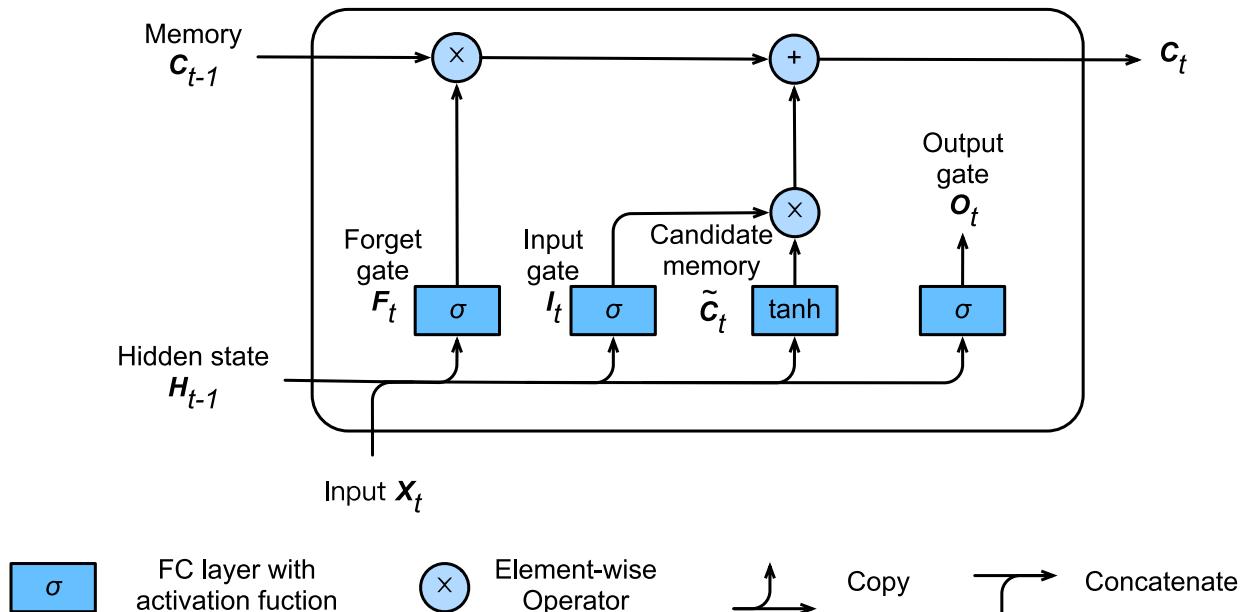


Fig. 10.9.3: Computation of memory cells in an LSTM. Here, the multiplication is carried out element-wise.

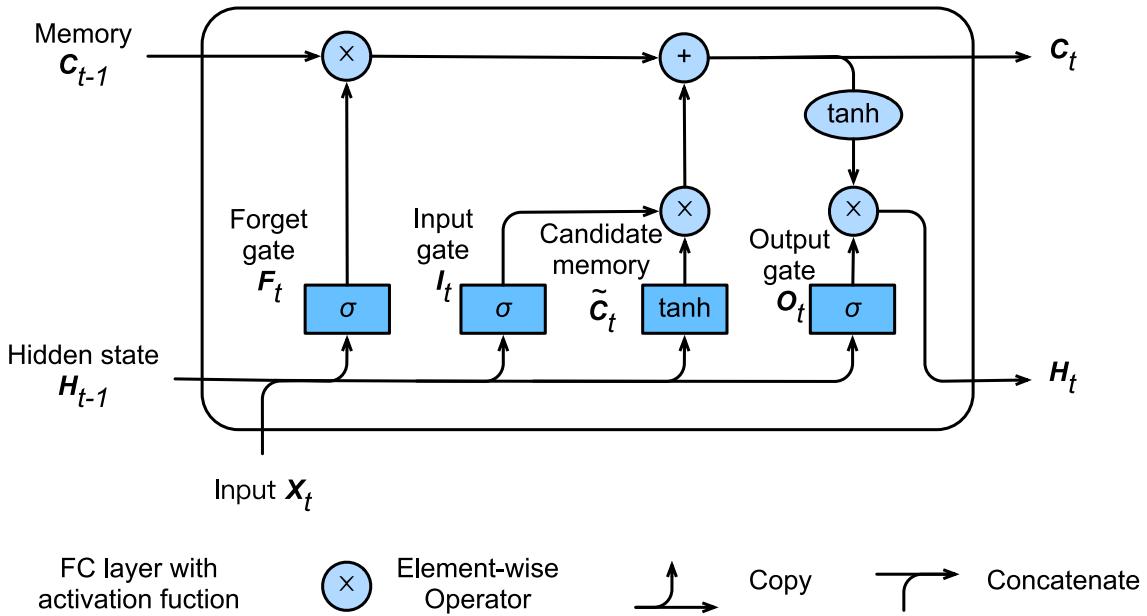


Fig. 10.9.4: Computation of the hidden state. Multiplication is element-wise.

## 10.9.2 Implementation from Scratch

Now it's time to implement an LSTM. We begin with a model built from scratch. As with the experiments in the previous sections we first need to load the data. We use *The Time Machine* for this.

```
import d2l
from mxnet import nd
from mxnet.gluon import rnn

batch_size, num_steps = 32, 35
train_iter, vocab = d2l.load_data_time_machine(batch_size, num_steps)
```

### Initialize Model Parameters

Next we need to define and initialize the model parameters. As previously, the hyperparameter `num_hiddens` defines the number of hidden units. We initialize weights with a Gaussian with 0.01 variance and we set the biases to 0.

```
def get_lstm_params(vocab_size, num_hiddens, ctx):
    num_inputs = num_outputs = vocab_size
    normal = lambda shape : nd.random.normal(scale=0.01, shape=shape, ctx=ctx)
    three = lambda : (normal((num_inputs, num_hiddens)),
                     normal((num_hiddens, num_hiddens)),
                     nd.zeros(num_hiddens, ctx=ctx))
    W_xi, W_hi, b_i = three() # Input gate parameters
    W_xf, W_hf, b_f = three() # Forget gate parameters
    W_xo, W_ho, b_o = three() # Output gate parameters
    W_xc, W_hc, b_c = three() # Candidate cell parameters
    # Output layer parameters
```

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```

W_hq = normal((num_hiddens, num_outputs))
b_q = nd.zeros(num_outputs, ctx=ctx)
# Create gradient
params = [W_xi, W_hi, b_i, W_xf, W_hf, b_f, W_xo, W_ho, b_o, W_xc, W_hc,
          b_c, W_hq, b_q]
for param in params:
    param.attach_grad()
return params

```

## Define the Model

In the initialization function, the hidden state of the LSTM needs to return an additional memory cell with a value of 0 and a shape of (batch size, number of hidden units). Hence we get the following state initialization.

```

def init_lstm_state(batch_size, num_hiddens, ctx):
    return (nd.zeros(shape=(batch_size, num_hiddens), ctx=ctx),
            nd.zeros(shape=(batch_size, num_hiddens), ctx=ctx))

```

The actual model is defined just like we discussed it before with three gates and an auxiliary memory cell. Note that only the hidden state is passed on to the output layer. The memory cells do not participate in the computation directly.

```

def lstm(inputs, state, params):
    [W_xi, W_hi, b_i, W_xf, W_hf, b_f, W_xo, W_ho, b_o, W_xc, W_hc, b_c,
     W_hq, b_q] = params
    (H, C) = state
    outputs = []
    for X in inputs:
        I = nd.sigmoid(nd.dot(X, W_xi) + nd.dot(H, W_hi) + b_i)
        F = nd.sigmoid(nd.dot(X, W_xf) + nd.dot(H, W_hf) + b_f)
        O = nd.sigmoid(nd.dot(X, W_xo) + nd.dot(H, W_ho) + b_o)
        C_tilda = nd.tanh(nd.dot(X, W_xc) + nd.dot(H, W_hc) + b_c)
        C = F * C + I * C_tilda
        H = O * C.tanh()
        Y = nd.dot(H, W_hq) + b_q
        outputs.append(Y)
    return nd.concat(*outputs, dim=0), (H, C)

```

## Training

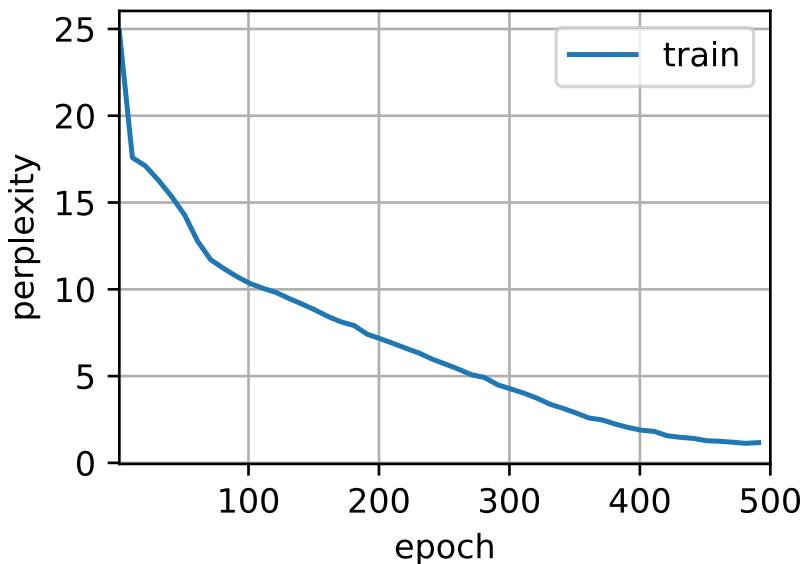
Again, we just train as before.

```

vocab_size, num_hiddens, ctx = len(vocab), 256, d2l.try_gpu()
num_epochs, lr = 500, 1
model = d2l.RNNModelScratch(len(vocab), num_hiddens, ctx, get_lstm_params,
                             init_lstm_state, lstm)
d2l.train_ch8(model, train_iter, vocab, lr, num_epochs, ctx)

```

```
Perplexity 1.1, 12173 tokens/sec on gpu(0)
time traveller smiled are you sure we can move freely inspace ri
traveller and what insies wo canstouice than shish we yould
```

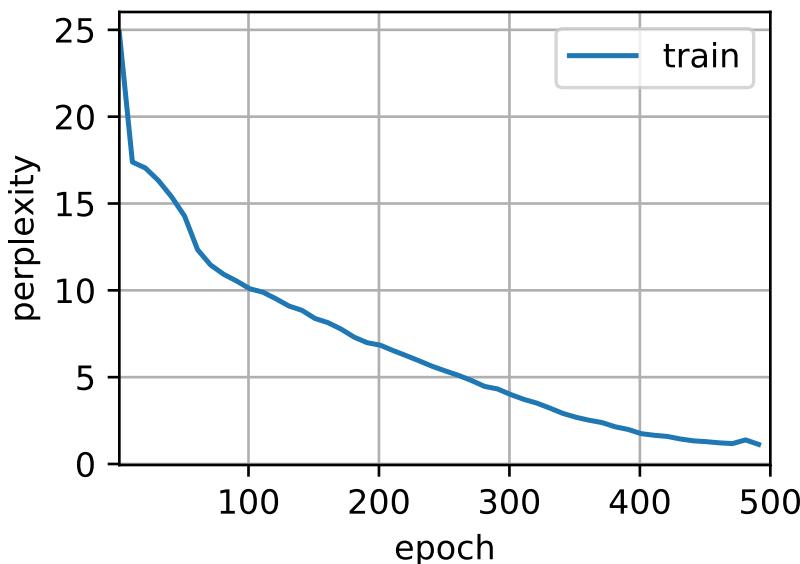


### 10.9.3 Concise Implementation

In Gluon, we can call the `LSTM` class in the `rnn` module directly to instantiate the model.

```
lstm_layer = rnn.LSTM(num_hiddens)
model = d2l.RNNModel(lstm_layer, len(vocab))
d2l.train_ch8(model, train_iter, vocab, lr, num_epochs, ctx)
```

```
Perplexity 1.1, 191353 tokens/sec on gpu(0)
time traveller it s against reason said filby what reason said
traveller so itwed ho ep and to egan tamof the other dimen
```



#### 10.9.4 Summary

- LSTMs have three types of gates: input, forget and output gates which control the flow of information.
- The hidden layer output of LSTM includes hidden states and memory cells. Only hidden states are passed into the output layer. Memory cells are entirely internal.
- LSTMs can help cope with vanishing and exploding gradients due to long range dependencies and short-range irrelevant data.
- In many cases LSTMs perform slightly better than GRUs but they are more costly to train and execute due to the larger latent state size.
- LSTMs are the prototypical latent variable autoregressive model with nontrivial state control. Many variants thereof have been proposed over the years, e.g. multiple layers, residual connections, different types of regularization.
- Training LSTMs and other sequence models is quite costly due to the long dependency of the sequence. Later we will encounter alternative models such as transformers that can be used in some cases.

#### 10.9.5 Exercises

1. Adjust the hyperparameters. Observe and analyze the impact on runtime, perplexity, and the generated output.
2. How would you need to change the model to generate proper words as opposed to sequences of characters?
3. Compare the computational cost for GRUs, LSTMs and regular RNNs for a given hidden dimension. Pay special attention to training and inference cost
4. Since the candidate memory cells ensure that the value range is between -1 and 1 using the tanh function, why does the hidden state need to use the tanh function again to ensure that the output value range is between -1 and 1?
5. Implement an LSTM for time series prediction rather than character sequences.

## 10.9.6 Scan the QR Code to Discuss<sup>150</sup>



## 10.10 Deep Recurrent Neural Networks

Up to now, we only discussed recurrent neural networks with a single unidirectional hidden layer. In it the specific functional form of how latent variables and observations interact was rather arbitrary. This isn't a big problem as long as we have enough flexibility to model different types of interactions. With a single layer, however, this can be quite challenging. In the case of the perceptron we fixed this problem by adding more layers. Within RNNs this is a bit more tricky, since we first need to decide how and where to add extra nonlinearity. Our discussion below focuses primarily on LSTMs but it applies to other sequence models, too.

- We could add extra nonlinearity to the gating mechanisms. That is, instead of using a single perceptron we could use multiple layers. This leaves the *mechanism* of the LSTM unchanged. Instead it makes it more sophisticated. This would make sense if we were led to believe that the LSTM mechanism describes some form of universal truth of how latent variable autoregressive models work.
- We could stack multiple layers of LSTMs on top of each other. This results in a mechanism that is more flexible, due to the combination of several simple layers. In particular, data might be relevant at different levels of the stack. For instance, we might want to keep high-level data about financial market conditions (bear or bull market) available at a high level, whereas at a lower level we only record shorter-term temporal dynamics.

Beyond all this abstract discussion it is probably easiest to understand the family of models we are interested in by reviewing the diagram below. It describes a deep recurrent neural network with  $L$  hidden layers. Each hidden state is continuously passed to the next time step of the current layer and the next layer of the current time step.

### 10.10.1 Functional Dependencies

At time step  $t$  we assume that we have a minibatch  $\mathbf{X}_t \in \mathbb{R}^{n \times d}$  (number of examples:  $n$ , number of inputs:  $d$ ). The hidden state of hidden layer  $\ell$  ( $\ell = 1, \dots, T$ ) is  $\mathbf{H}_t^{(\ell)} \in \mathbb{R}^{n \times h}$  (number of hidden units:  $h$ ), the output layer variable is  $\mathbf{O}_t \in \mathbb{R}^{n \times q}$  (number of outputs:  $q$ ) and a hidden layer activation function  $f_l$  for layer  $l$ . We compute the hidden state of layer 1 as before, using  $\mathbf{X}_t$  as input. For all subsequent layers the hidden state of the previous layer is used in its place.

$$\begin{aligned}\mathbf{H}_t^{(1)} &= f_1\left(\mathbf{X}_t, \mathbf{H}_{t-1}^{(1)}\right) \\ \mathbf{H}_t^{(l)} &= f_l\left(\mathbf{H}_t^{(l-1)}, \mathbf{H}_{t-1}^{(l)}\right)\end{aligned}\tag{10.10.1}$$

Finally, the output of the output layer is only based on the hidden state of hidden layer  $L$ . We use the output function  $g$  to address this:

$$\mathbf{O}_t = g\left(\mathbf{H}_t^{(L)}\right)\tag{10.10.2}$$

<sup>150</sup> <https://discuss.mxnet.io/t/2368>

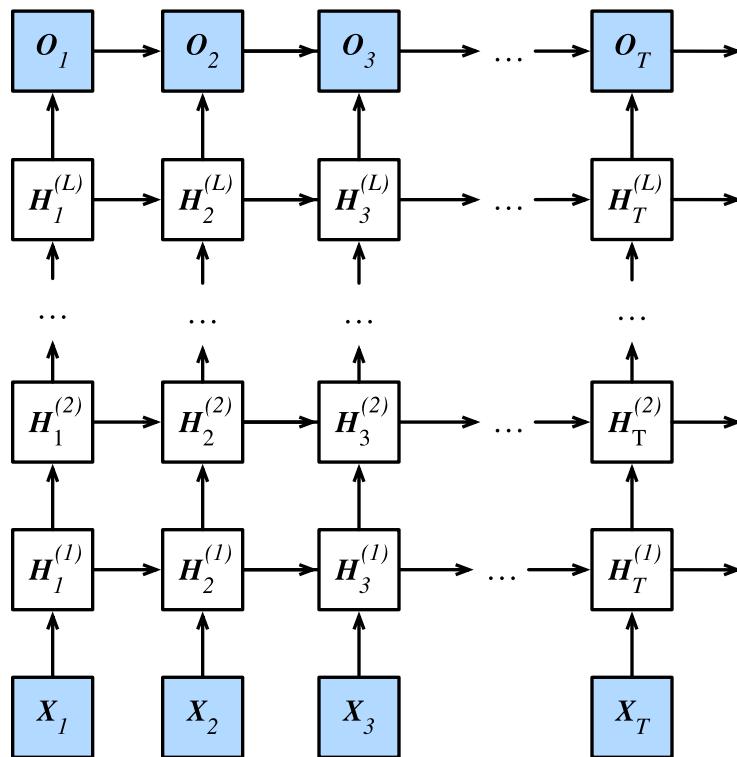


Fig. 10.10.1: Architecture of a deep recurrent neural network.

Just as with multilayer perceptrons, the number of hidden layers  $L$  and number of hidden units  $h$  are hyper parameters. In particular, we can pick a regular RNN, a GRU or an LSTM to implement the model.

### 10.10.2 Concise Implementation

Fortunately many of the logistical details required to implement multiple layers of an RNN are readily available in Gluon. To keep things simple we only illustrate the implementation using such built-in functionality. The code is very similar to the one we used previously for LSTMs. In fact, the only difference is that we specify the number of layers explicitly rather than picking the default of a single layer. Let's begin by importing the appropriate modules and data.

```
import d2l
from mxnet import nd
from mxnet.gluon import rnn

batch_size, num_steps = 32, 35
train_iter, vocab = d2l.load_data_time_machine(batch_size, num_steps)
```

The architectural decisions (parameters, etc.) are very similar to those of previous sections. We pick the same number of inputs and outputs as we have distinct tokens, i.e. `vocab_size`. The number of hidden units is still 256. The only difference is that we now select a nontrivial number of layers `num_layers = 2`. Since the model is somewhat slower to train we use 3000 iterations.

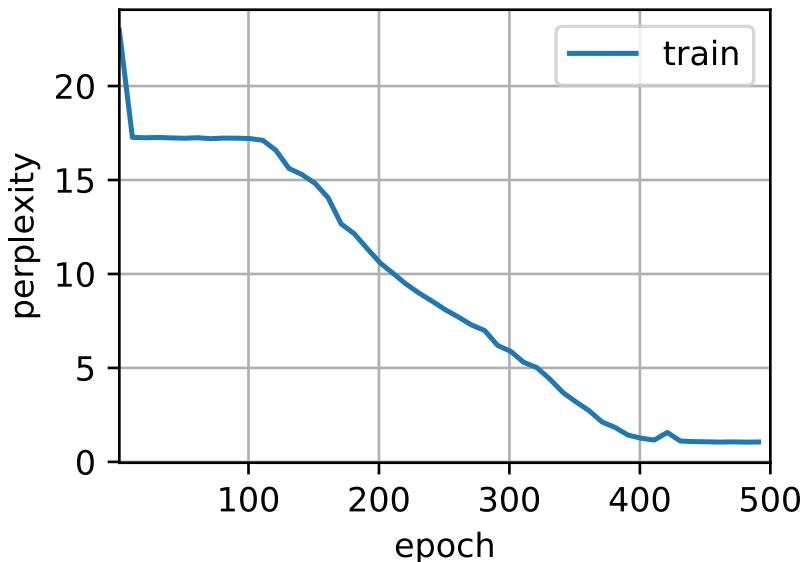
```
vocab_size, num_hiddens, num_layers, ctx = len(vocab), 256, 2, d2l.try_gpu()
lstm_layer = rnn.LSTM(num_hiddens, num_layers)
model = d2l.RNNModel(lstm_layer, len(vocab))
```

### 10.10.3 Training

The actual invocation logic is identical to before. The only difference is that we now instantiate two layers with LSTMs. This rather more complex architecture and the large number of epochs slow down training considerably.

```
num_epochs, lr = 500, 2
d2l.train_ch8(model, train_iter, vocab, lr, num_epochs, ctx)
```

```
Perplexity 1.0, 131418 tokens/sec on gpu(0)
time traveller it s against reason said filby what reason said
traveller it s against reason said filby what reason said
```



### 10.10.4 Summary

- In deep recurrent neural networks, hidden state information is passed to the next time step of the current layer and the next layer of the current time step.
- There exist many different flavors of deep RNNs, such as LSTMs, GRUs or regular RNNs. Conveniently these models are all available as parts of the `rnn` module in Gluon.
- Initialization of the models requires care. Overall, deep RNNs require considerable amount of work (learning rate, clipping, etc) to ensure proper convergence.

### 10.10.5 Exercises

1. Try to implement a two-layer RNN from scratch using the single layer implementation we discussed in [Section 10.5](#).
2. Replace the LSTM by a GRU and compare the accuracy.
3. Increase the training data to include multiple books. How low can you go on the perplexity scale?
4. Would you want to combine sources of different authors when modeling text? Why is this a good idea? What could go wrong?

### 10.10.6 Scan the QR Code to Discuss<sup>151</sup>



## 10.11 Bidirectional Recurrent Neural Networks

So far we assumed that our goal is to model the next word given what we've seen so far, e.g. in the context of a time series or in the context of a language model. While this is a typical scenario, it is not the only one we might encounter. To illustrate the issue, consider the following three tasks of filling in the blanks in a text:

1. I am \_\_\_\_\_
2. I am \_\_\_\_\_ very hungry.
3. I am \_\_\_\_\_ very hungry, I could eat half a pig.

Depending on the amount of information available we might fill the blanks with very different words such as '*happy*', '*not*', and '*very*'. Clearly the end of the phrase (if available) conveys significant information about which word to pick. A sequence model that is incapable of taking advantage of this will perform poorly on related tasks. For instance, to do well in named entity recognition (e.g. to recognize whether *Green* refers to *Mr. Green* or to the color) longer-range context is equally vital. To get some inspiration for addressing the problem let's take a detour to graphical models.

### 10.11.1 Dynamic Programming

This section serves to *illustrate* the problem. The specific technical details do not matter for understanding the deep learning counterpart but they help in motivating why one might use deep learning and why one might pick specific architectures.

If we want to solve the problem using graphical models we could for instance design a latent variable model as follows: we assume that there exists some latent variable  $h_t$  which governs the emissions  $x_t$  that we observe via  $p(x_t|h_t)$ . Moreover, the transitions  $h_t \rightarrow h_{t+1}$  are given by some state transition probability  $p(h_t|h_{t-1})$ . The graphical model then looks as follows:

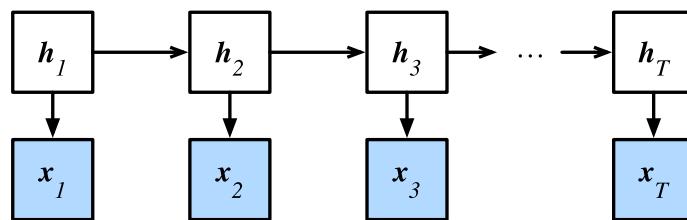


Fig. 10.11.1: Hidden Markov Model.

<sup>151</sup> <https://discuss.mxnet.io/t/2369>

For a sequence of  $T$  observations we have thus the following joint probability distribution over observed and hidden states:

$$p(x, h) = p(h_1)p(x_1|h_1)\prod_{i=2}^T p(h_t|h_{t-1})p(x_t|h_t) \quad (10.11.1)$$

Now assume that we observe all  $x_i$  with the exception of some  $x_j$  and it is our goal to compute  $p(x_j|x^{-j})$ . To accomplish this we need to sum over all possible choices of  $h = (h_1, \dots, h_T)$ . In case  $h_i$  can take on  $k$  distinct values this means that we need to sum over  $k^T$  terms - mission impossible! Fortunately there's an elegant solution for this: dynamic programming. To see how it works consider summing over the first two hidden variable  $h_1$  and  $h_2$ . This yields:

$$\begin{aligned} p(x) &= \sum_h p(h_1)p(x_1|h_1)\prod_{i=2}^T p(h_t|h_{t-1})p(x_t|h_t) \\ &= \sum_{h_2, \dots, h_T} \underbrace{\left[ \sum_{h_1} p(h_1)p(x_1|h_1)p(h_2|h_1) \right]}_{=: \pi_2(h_2)} p(x_2|h_2)\prod_{i=2}^T p(h_t|h_{t-1})p(x_t|h_t) \\ &= \sum_{h_3, \dots, h_T} \underbrace{\left[ \sum_{h_2} \pi_2(h_2)p(x_2|h_2)p(h_3|h_2) \right]}_{=: \pi_3(h_3)} p(x_3|h_3)\prod_{i=3}^T p(h_t|h_{t-1})p(x_t|h_t) \end{aligned} \quad (10.11.2)$$

In general we have the *forward* recursion

$$\pi_{t+1}(h_{t+1}) = \sum_{h_t} \pi_t(h_t)p(x_t|h_t)p(h_{t+1}|h_t) \quad (10.11.3)$$

The recursion is initialized as  $\pi_1(h_1) = p(h_1)$ . In abstract terms this can be written as  $\pi_{t+1} = f(\pi_t, x_t)$ , where  $f$  is some learned function. This looks very much like the update equation in the hidden variable models we discussed so far in the context of RNNs. Entirely analogously to the forward recursion we can also start a backwards recursion. This yields:

$$\begin{aligned} p(x) &= \sum_h \prod_{i=1}^{T-1} p(h_t|h_{t-1})p(x_t|h_t) \cdot p(h_T|h_{T-1})p(x_T|h_T) \\ &= \sum_{h_1, \dots, h_{T-1}} \prod_{i=1}^{T-1} p(h_t|h_{t-1})p(x_t|h_t) \cdot \underbrace{\left[ \sum_{h_T} p(h_T|h_{T-1})p(x_T|h_T) \right]}_{=: \rho_{T-1}(h_{T-1})} \\ &= \sum_{h_1, \dots, h_{T-2}} \prod_{i=1}^{T-2} p(h_t|h_{t-1})p(x_t|h_t) \cdot \underbrace{\left[ \sum_{h_{T-1}} p(h_{T-1}|h_{T-2})p(x_{T-1}|h_{T-1}) \right]}_{=: \rho_{T-2}(h_{T-2})} \end{aligned} \quad (10.11.4)$$

We can thus write the *backward* recursion as

$$\rho_{t-1}(h_{t-1}) = \sum_{h_t} p(h_t|h_{t-1})p(x_t|h_t) \quad (10.11.5)$$

with initialization  $\rho_T(h_T) = 1$ . These two recursions allow us to sum over  $T$  variables in  $O(kT)$  (linear) time over all values of  $(h_1, \dots, h_T)$  rather than in exponential time. This is one of the great benefits of probabilistic inference with graphical models. It is a very special instance of the [Generalized Distributive Law](#)<sup>152</sup> proposed

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<sup>152</sup> <https://authors.library.caltech.edu/1541/1/AJlieetit00.pdf>

in 2000 by Aji and McEliece. Combining both forward and backward pass we are able to compute

$$p(x_j|x_{-j}) \propto \sum_{h_j} \pi_j(h_j) \rho_j(h_j) p(x_j|h_j). \quad (10.11.6)$$

Note that in abstract terms the backward recursion can be written as  $\rho_{t-1} = g(\rho_t, x_t)$ , where  $g$  is some learned function. Again, this looks very much like an update equation, just running backwards unlike what we've seen so far in RNNs. And, indeed, HMMs benefit from knowing future data when it is available. Signal processing scientists distinguish between the two cases of knowing and not knowing future observations as filtering vs. smoothing. See e.g. the introductory chapter of the book by [Doucet, de Freitas and Gordon, 2001](#)<sup>153</sup> on Sequential Monte Carlo algorithms for more detail.

### 10.11.2 Bidirectional Model

If we want to have a mechanism in RNNs that offers comparable look-ahead ability as in HMMs we need to modify the recurrent net design we've seen so far. Fortunately this is easy (conceptually). Instead of running an RNN only in forward mode starting from the first symbol we start another one from the last symbol running back to front. Bidirectional recurrent neural networks add a hidden layer that passes information in a backward direction to more flexibly process such information. The figure below illustrates the architecture of a bidirectional recurrent neural network with a single hidden layer.

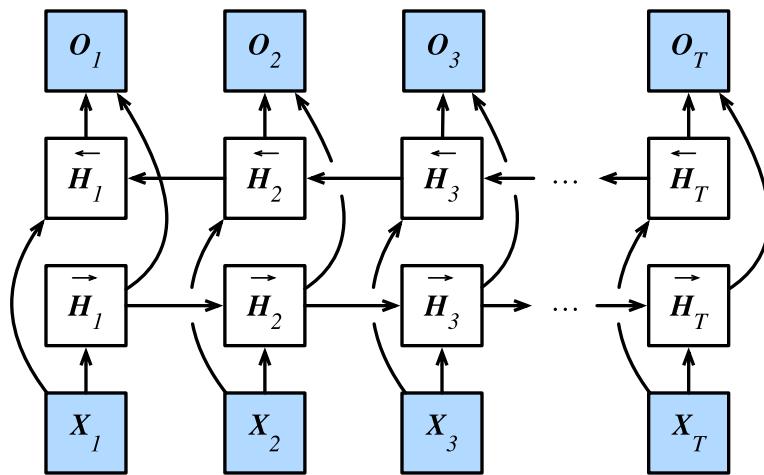


Fig. 10.11.2: Architecture of a bidirectional recurrent neural network.

In fact, this is not too dissimilar to the forward and backward recurrences we encountered above. The main distinction is that in the previous case these equations had a specific statistical meaning. Now they're devoid of such easily accessible interpretation and we can just treat them as generic functions. This transition epitomizes many of the principles guiding the design of modern deep networks - use the type of functional dependencies common to classical statistical models and use them in a generic form.

#### Definition

Bidirectional RNNs were introduced by Schuster and Paliwal, 1997<sup>154</sup>. For a detailed discussion of the various architectures see also the paper by Graves and Schmidhuber, 2005<sup>155</sup>. Let's look at the specifics of such a network. For a given time step  $t$ , the mini-batch input is  $\mathbf{X}_t \in \mathbb{R}^{n \times d}$  (number of examples:  $n$ , number

<sup>153</sup> [https://www.stats.ox.ac.uk/~doucet/doucet\\_defreitas\\_gordon\\_smcbokintro.pdf](https://www.stats.ox.ac.uk/~doucet/doucet_defreitas_gordon_smcbokintro.pdf)

<sup>154</sup> <https://ieeexplore.ieee.org/abstract/document/650093>

<sup>155</sup> <https://www.sciencedirect.com/science/article/pii/S0893608005001206>

of inputs:  $d$ ) and the hidden layer activation function is  $\phi$ . In the bidirectional architecture: We assume that the forward and backward hidden states for this time step are  $\vec{\mathbf{H}}_t \in \mathbb{R}^{n \times h}$  and  $\overleftarrow{\mathbf{H}}_t \in \mathbb{R}^{n \times h}$  respectively. Here  $h$  indicates the number of hidden units. We compute the forward and backward hidden state updates as follows:

$$\begin{aligned}\vec{\mathbf{H}}_t &= \phi(\mathbf{X}_t \mathbf{W}_{xh}^{(f)} + \vec{\mathbf{H}}_{t-1} \mathbf{W}_{hh}^{(f)} + \mathbf{b}_h^{(f)}), \\ \overleftarrow{\mathbf{H}}_t &= \phi(\mathbf{X}_t \mathbf{W}_{xh}^{(b)} + \overleftarrow{\mathbf{H}}_{t+1} \mathbf{W}_{hh}^{(b)} + \mathbf{b}_h^{(b)}),\end{aligned}\quad (10.11.7)$$

Here, the weight parameters  $\mathbf{W}_{xh}^{(f)} \in \mathbb{R}^{d \times h}$ ,  $\mathbf{W}_{hh}^{(f)} \in \mathbb{R}^{h \times h}$ ,  $\mathbf{W}_{xh}^{(b)} \in \mathbb{R}^{d \times h}$ , and  $\mathbf{W}_{hh}^{(b)} \in \mathbb{R}^{h \times h}$  and bias parameters  $\mathbf{b}_h^{(f)} \in \mathbb{R}^{1 \times h}$  and  $\mathbf{b}_h^{(b)} \in \mathbb{R}^{1 \times h}$  are all model parameters.

Then we concatenate the forward and backward hidden states  $\vec{\mathbf{H}}_t$  and  $\overleftarrow{\mathbf{H}}_t$  to obtain the hidden state  $\mathbf{H}_t \in \mathbb{R}^{n \times 2h}$  and input it to the output layer. In deep bidirectional RNNs the information is passed on as *input* to the next bidirectional layer. Lastly, the output layer computes the output  $\mathbf{O}_t \in \mathbb{R}^{n \times q}$  (number of outputs:  $q$ ):

$$\mathbf{O}_t = \mathbf{H}_t \mathbf{W}_{hq} + \mathbf{b}_q, \quad (10.11.8)$$

Here, the weight parameter  $\mathbf{W}_{hq} \in \mathbb{R}^{2h \times q}$  and bias parameter  $\mathbf{b}_q \in \mathbb{R}^{1 \times q}$  are the model parameters of the output layer. The two directions can have different numbers of hidden units.

## Computational Cost and Applications

One of the key features of a bidirectional RNN is that information from both ends of the sequence is used to estimate the output. That is, we use information from future and past observations to predict the current one (a smoothing scenario). In the case of language models this isn't quite what we want. After all, we don't have the luxury of knowing the next to next symbol when predicting the next one. Hence, if we were to use a bidirectional RNN naively we wouldn't get very good accuracy: during training we have past and future data to estimate the present. During test time we only have past data and thus poor accuracy (we will illustrate this in an experiment below).

To add insult to injury bidirectional RNNs are also exceedingly slow. The main reason for this is that they require both a forward and a backward pass and that the backward pass is dependent on the outcomes of the forward pass. Hence gradients will have a very long dependency chain.

In practice bidirectional layers are used very sparingly and only for a narrow set of applications, such as filling in missing words, annotating tokens (e.g. for named entity recognition), or encoding sequences wholesale as a step in a sequence processing pipeline (e.g. for machine translation). In short, handle with care!

## Training a BLSTM for the Wrong Application

If we were to ignore all advice regarding the fact that bidirectional LSTMs use past and future data and simply apply it to language models we will get estimates with acceptable perplexity. Nonetheless the ability of the model to predict future symbols is severely compromised as the example below illustrates. Despite reasonable perplexity numbers it only generates gibberish even after many iterations. We include the code below as a cautionary example against using them in the wrong context.

```
import d2l
from mxnet import nd
from mxnet.gluon import rnn

# Load data
batch_size, num_steps = 32, 35
```

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```

train_iter, vocab = d2l.load_data_time_machine(batch_size, num_steps)
# Define model
vocab_size, num_hiddens, num_layers, ctx = len(vocab), 256, 2, d2l.try_gpu()
lstm_layer = rnn.LSTM(num_hiddens, num_layers, bidirectional=True)
model = d2l.RNNModel(lstm_layer, len(vocab))
# Train
num_epochs, lr = 500, 1
d2l.train_ch8(model, train_iter, vocab, lr, num_epochs, ctx)

```

```

Perplexity 1.2, 79229 tokens/sec on gpu(0)
time travellererererererererererererererererer
travellererererererererererererererererer

```

The output is clearly unsatisfactory for the reasons described above. For a discussion of more effective uses of bidirectional models see e.g. the sentiment classification in Section 15.9.

### 10.11.3 Summary

- In bidirectional recurrent neural networks, the hidden state for each time step is simultaneously determined by the data prior and after the current timestep.
- Bidirectional RNNs bear a striking resemblance with the forward-backward algorithm in graphical models.
- Bidirectional RNNs are mostly useful for sequence embedding and the estimation of observations given bidirectional context.
- Bidirectional RNNs are very costly to train due to long gradient chains.

### 10.11.4 Exercises

1. If the different directions use a different number of hidden units, how will the shape of  $\mathbf{H}_t$  change?
2. Design a bidirectional recurrent neural network with multiple hidden layers.
3. Implement a sequence classification algorithm using bidirectional RNNs. Hint - use the RNN to embed each word and then aggregate (average) all embedded outputs before sending the output into an MLP for classification. For instance, if we have  $(\mathbf{o}_1, \mathbf{o}_2, \mathbf{o}_3)$  we compute  $\bar{\mathbf{o}} = \frac{1}{3} \sum_i \mathbf{o}_i$  first and then use the latter for sentiment classification.

### 10.11.5 Scan the QR Code to Discuss<sup>156</sup>



<sup>156</sup> <https://discuss.mxnet.io/t/2370>

## 10.12 Machine Translation and Data Sets

So far we see how to use recurrent neural networks for language models, in which we predict the next token given all previous tokens in an article. Now let's have a look at a different application, machine translation, whose predict output is no longer a single token, but a list of tokens.

Machine translation (MT) refers to the automatic translation of a segment of text from one language to another. Solving this problem with neural networks is often called neural machine translation (NMT). Compared to language models (Section 10.3), in which the corpus only contains a single language, machine translation data set has at least two languages, the source language and the target language. In addition, each sentence in the source language is mapped to the according translation in the target language. Therefore, the data preprocessing for machine translation data is different to the one for language models. This section is dedicated to demonstrate how to pre-process such a data set and then load into a set of mini-batches.

```
import collections
import d2l
import zipfile

from mxnet import nd, gluon
```

### 10.12.1 Read and Pre-process Data

We first download a dataset that contains a set of English sentences with the corresponding French translations. As can be seen that each line contains a English sentence with its French translation, which are separated by a TAB.

```
# Save to the d2l package.
def read_data_nmt():
    fname = gluon.utils.download('http://data.mxnet.io/data/fra-eng.zip')
    with zipfile.ZipFile(fname, 'r') as f:
        return f.read('fra.txt').decode("utf-8")

raw_text = read_data_nmt()
print(raw_text[0:106])
```

Go.	Va !
Hi.	Salut !
Run!	Cours !
Run!	Courez !
Who?	Qui ?
Wow!	Ça alors !
Fire!	Au feu !
Help!	À l'aide !

We perform several preprocessing steps on the raw text data, including ignoring cases, replacing UTF-8 non-breaking space with space, and adding space between words and punctuation marks.

```
# Save to the d2l package.
def preprocess_nmt(text):
    text = text.replace('\u202f', ' ').replace('\xa0', ' ')
    no_space = lambda char, prev_char: (
        True if char in (' ',',','!',',.') and prev_char != ' ' else False)
```

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```

out = [' '+char if i > 0 and no_space(char, text[i-1]) else char
       for i, char in enumerate(text.lower())]
return ''.join(out)

text = preprocess_nmt(raw_text)
print(text[0:95])

```

```

go .      va !
hi .      salut !
run !     cours !
run !     courez !
who?      qui ?
wow !    ça alors !
fire !   au feu !

```

### 10.12.2 Tokenization

Different to using character tokens in Section 10.3, here a token is either a word or a punctuation mark. The following function tokenize the text data to return `source` and `target`. Each one is a list of token list, with `source[i]` is the i-th sentence in the source language and `target[i]` is the i-th sentence in the target language. To make the latter training faster, we sample the first `num_examples` sentences pairs.

```

# Save to the d2l package.
def tokenize_nmt(text, num_examples = None):
    source, target = [], []
    for i, line in enumerate(text.split('\n')):
        if num_examples and i > num_examples: break
        parts = line.split('\t')
        if len(parts) == 2:
            source.append(parts[0].split(' '))
            target.append(parts[1].split(' '))
    return source, target

source, target = tokenize_nmt(text)
source[0:3], target[0:3]

```

```

([['go', '.'], ['hi', '.'], ['run', '!']],
[['va', '!'], ['salut', '!'], ['cours', '!']])

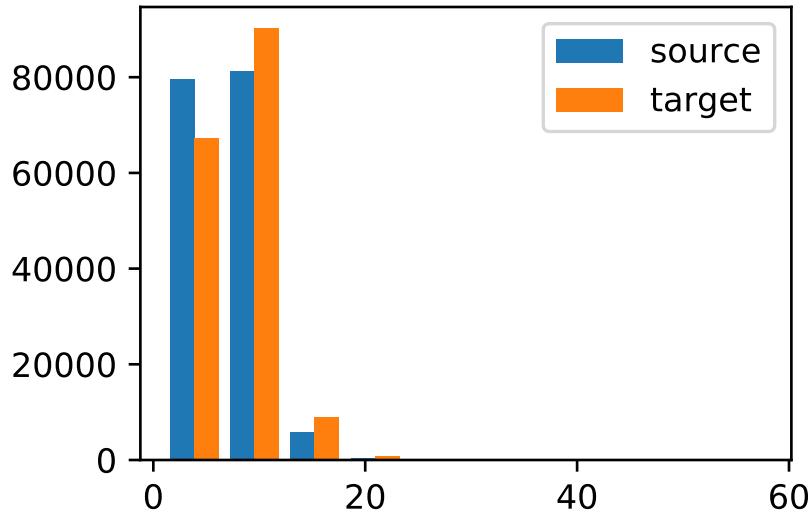
```

We visualize the histogram of the number of tokens per sentence the following figure. As can be seen that a sentence in average contains 5 tokens, and most of them have less than 10 tokens.

```

d2l.set_figsize((3.5, 2.5))
d2l.plt.hist([[len(l) for l in source], [len(l) for l in target]],
            label=['source', 'target'])
d2l.plt.legend(loc='upper right');

```



### 10.12.3 Vocabulary

Since the tokens in the source language could be different to the ones in the target language, we need to build a vocabulary for each of them. Since we are using words instead of characters as tokens, it makes the vocabulary size significantly large. Here we map every token that appears less than 3 times into the `<unk>` token Section 10.2. In addition, we need other special tokens such as padding and sentence beginnings.

```
src_vocab = d2l.Vocab(source, min_freq=3, use_special_tokens=True)
len(src_vocab)
```

9140

### 10.12.4 Load Dataset

In language models, each example is a `num_steps` length sequence from the corpus, which may be a segment of a sentence, or span over multiple sentences. In machine translation, an example should contain a pair of source sentence and target sentence. These sentences might have different lengths, while we need same length examples to form a mini-batch.

One way to solve this problem is that if a sentence is longer than `num_steps`, we trim it's length, otherwise pad with a special `<pad>` token to meet the length. Therefore we could transform any sentence to a fixed length.

```
# Save to the d2l package.
def trim_pad(line, num_steps, padding_token):
    if len(line) > num_steps: return line[:num_steps] # Trim
    return line + [padding_token] * (num_steps - len(line)) # Pad

trim_pad(src_vocab[source[0]], 10, src_vocab.pad)
```

[47, 4, 0, 0, 0, 0, 0, 0, 0]

Now we can convert a list of sentences into an `(num_example, num_steps)` index array. We also record the length of each sentence without the padding tokens, called *valid length*, which might be used by some

models. In addition, we add the special “<bos>” and “<eos>” tokens to the target sentences so that our model will know the signals for starting and ending predicting.

```
# Save to the d2l package.
def build_array(lines, vocab, num_steps, is_source):
    lines = [vocab[1] for l in lines]
    if not is_source:
        lines = [[vocab.bos] + l + [vocab.eos] for l in lines]
    array = nd.array(trim_pad(l, num_steps, vocab.pad) for l in lines))
    valid_len = (array != vocab.pad).sum(axis=1)
    return array, valid_len
```

Then we can construct mini-batches based on these arrays.

### 10.12.5 Put All Things Together

Finally, we define the function `load_data_nmt` to return the data iterator with the vocabularies for source language and target language.

```
# Save to the d2l package.
def load_data_nmt(batch_size, num_steps, num_examples=1000):
    text = preprocess_nmt(read_data_nmt())
    source, target = tokenize_nmt(text, num_examples)
    src_vocab = d2l.Vocab(source, min_freq=3, use_special_tokens=True)
    tgt_vocab = d2l.Vocab(target, min_freq=3, use_special_tokens=True)
    src_array, src_valid_len = build_array(
        source, src_vocab, num_steps, True)
    tgt_array, tgt_valid_len = build_array(
        target, tgt_vocab, num_steps, False)
    data_arrays = (src_array, src_valid_len, tgt_array, tgt_valid_len)
    data_iter = d2l.load_array(data_arrays, batch_size)
    return src_vocab, tgt_vocab, data_iter
```

Let’s read the first batch.

```
src_vocab, tgt_vocab, train_iter = load_data_nmt(batch_size=2, num_steps=8)
for X, X_vlen, Y, Y_vlen, in train_iter:
    print('X =', X.astype('int32'), '\nValid lengths for X =', X_vlen,
          '\nY =', Y.astype('int32'), '\nValid lengths for Y =', Y_vlen)
    break
```

```
X =
[[ 89 173   4   0   0   0   0   0]
 [ 7  86   4   0   0   0   0   0]]
<NDArray 2x8 @cpu(0)>
Valid lengths for X =
[3. 3.]
<NDArray 2 @cpu(0)>
Y =
[[ 1   3   4   2   0   0   0   0]
 [ 1   6   7 124   4   2   0   0]]
<NDArray 2x8 @cpu(0)>
Valid lengths for Y =
```

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```
[4. 6.]
<NDArray 2 @cpu(0)>
```

## 10.12.6 Summary

## 10.13 Encoder-Decoder Architecture

The encoder-decoder architecture is a neural network design pattern. In this architecture, the network is partitioned into two parts, the encoder and the decoder. The encoder's role is encoding the inputs into state, which often contains several tensors. Then the state is passed into the decoder to generate the outputs. In machine translation, the encoder transforms a source sentence, e.g. “Hello world.”, into state, e.g. a vector, that captures its semantic information. The decoder then uses this state to generate the translated target sentence, e.g. “Bonjour le monde.”.

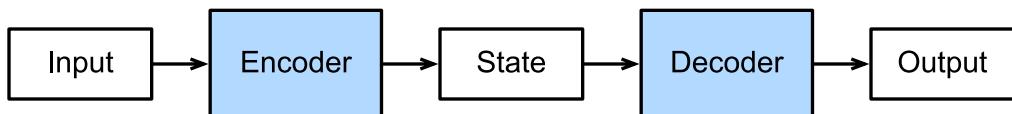


Fig. 10.13.1: The encoder-decoder architecture.

In this section, we will show an interface to implement this encoder-decoder architecture.

```
from mxnet.gluon import nn
```

### 10.13.1 Encoder

The encoder is a normal neural network that takes inputs, e.g. a source sentence, to return outputs.

```
# Save to the d2l package.
class Encoder(nn.Block):
    """The base encoder interface for the encoder-decoder architecture."""
    def __init__(self, **kwargs):
        super(Encoder, self).__init__(**kwargs)

    def forward(self, X):
        raise NotImplementedError
```

### 10.13.2 Decoder

The decoder has an additional method `init_state` to parse the outputs of the encoder with possible additional information, e.g. the valid lengths of inputs, to return the state it needs. In the forward method, the decoder takes both inputs, e.g. a target sentence, and the state. It returns outputs, with potentially modified state if the encoder contains RNN layers.

```
# Save to the d2l package.
class Decoder(nn.Block):
    """The base decoder interface for the encoder-decoder architecture."""

```

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```

def __init__(self, **kwargs):
    super(Decoder, self).__init__(**kwargs)

def init_state(self, enc_outputs, *args):
    raise NotImplementedError

def forward(self, X, state):
    raise NotImplementedError

```

### 10.13.3 Model

The encoder-decoder model contains both an encoder and decoder. We implement its forward method for training. It takes both encoder inputs and decoder inputs, with optional additional information. During computation, it first computes encoder outputs to initialize the decoder state, and then returns the decoder outputs.

```

# Save to the d2l package.
class EncoderDecoder(nn.Block):
    """The base class for the encoder-decoder architecture."""
    def __init__(self, encoder, decoder, **kwargs):
        super(EncoderDecoder, self).__init__(**kwargs)
        self.encoder = encoder
        self.decoder = decoder

    def forward(self, enc_X, dec_X, *args):
        enc_outputs = self.encoder(enc_X, *args)
        dec_state = self.decoder.init_state(enc_outputs, *args)
        return self.decoder(dec_X, dec_state)

```

### 10.13.4 Summary

## 10.14 Sequence to Sequence

The sequence-to-sequence (seq2seq) model is based on the encoder-decoder architecture to generate a sequence output for a sequence input. Both the encoder and the decoder use recurrent neural networks to handle sequence inputs. The hidden state of the encoder is used directly to initialize the decoder hidden state to pass information from the encoder to the decoder.

The layers in the encoder and the decoder are illustrated in the following figure.

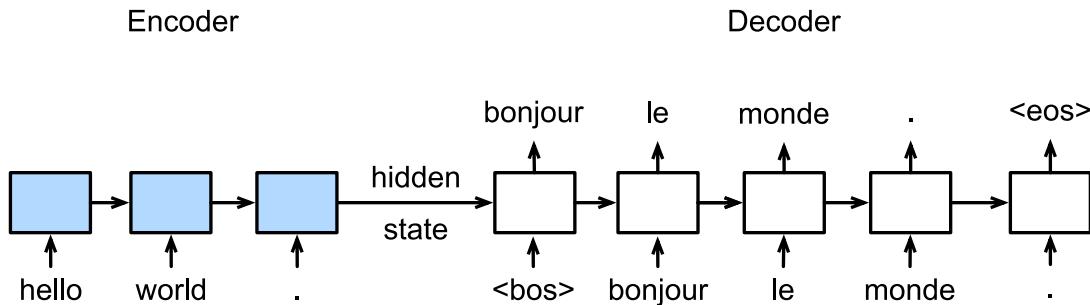
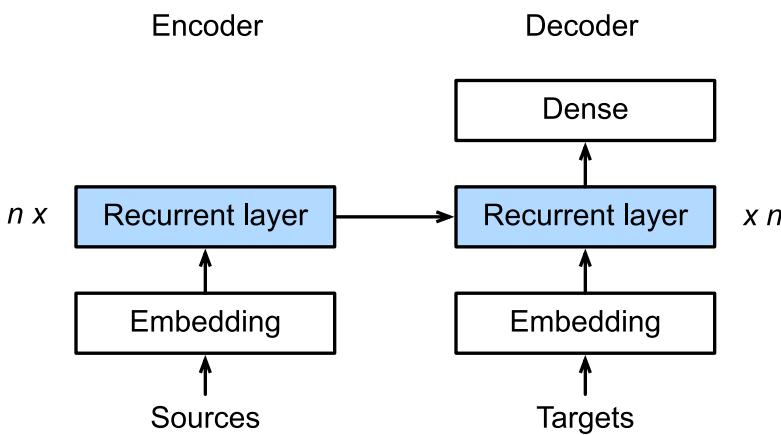


Fig. 10.14.1: The sequence to sequence model architecture.



In this section we will implement the seq2seq model to train on the machine translation dataset.

```
from mxnet import nd, init, gluon, autograd
from mxnet.gluon import nn, rnn
import d2l
```

### 10.14.1 Encoder

In the encoder, we use the word embedding layer to obtain a feature index from the word index of the input language and then input it into a multi-level LSTM recurrent unit. The input for the encoder is a batch of sequences, which is 2-D tensor with shape (batch size, sequence length). It outputs both the LSTM outputs, e.g the hidden state, for each time step and the hidden state and memory cell of the last time step.

```
# Save to the d2l package.
class Seq2SeqEncoder(d2l.Encoder):
    def __init__(self, vocab_size, embed_size, num_hiddens, num_layers,
                 dropout=0, **kwargs):
        super(Seq2SeqEncoder, self).__init__(**kwargs)
        self.embedding = nn.Embedding(vocab_size, embed_size)
        self.rnn = rnn.LSTM(num_hiddens, num_layers, dropout=dropout)

    def forward(self, X, *args):
        X = self.embedding(X) # X shape: (batch_size, seq_len, embed_size)
```

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```
X = X.swapaxes(0, 1) # RNN needs first axes to be time
state = self.rnn.begin_state(batch_size=X.shape[1], ctx=X.context)
out, state = self.rnn(X, state)
# The shape of out is (seq_len, batch_size, num_hiddens).
# state contains the hidden state and the memory cell
# of the last time step, the shape is (num_layers, batch_size, num_hiddens)
return out, state
```

Next, we will create a mini-batch sequence input with a batch size of 4 and 7 time steps. We assume the number of hidden layers of the LSTM unit is 2 and the number of hidden units is 16. The output shape returned by the encoder after performing forward calculation on the input is (number of time steps, batch size, number of hidden units). The shape of the multi-layer hidden state of the gated recurrent unit in the final time step is (number of hidden layers, batch size, number of hidden units). For the gated recurrent unit, the `state` list contains only one element, which is the hidden state. If long short-term memory is used, the `state` list will also contain another element, which is the memory cell.

```
encoder = Seq2SeqEncoder(vocab_size=10, embed_size=8,
                           num_hiddens=16, num_layers=2)
encoder.initialize()
X = nd.zeros((4, 7))
output, state = encoder(X)
output.shape, len(state), state[0].shape, state[1].shape
```

```
((7, 4, 16), 2, (2, 4, 16), (2, 4, 16))
```

### 10.14.2 Decoder

We directly use the hidden state of the encoder in the final time step as the initial hidden state of the decoder. This requires that the encoder and decoder RNNs have the same numbers of layers and hidden units.

The forward calculation of the decoder is similar to the encoder's. The only difference is we add a dense layer with the hidden size to be the vocabulary size to output the predicted confidence score for each word.

```
# Save to the d2l package.
class Seq2SeqDecoder(d2l.Decoder):
    def __init__(self, vocab_size, embed_size, num_hiddens, num_layers,
                 dropout=0, **kwargs):
        super(Seq2SeqDecoder, self).__init__(**kwargs)
        self.embedding = nn.Embedding(vocab_size, embed_size)
        self.rnn = rnn.LSTM(num_hiddens, num_layers, dropout=dropout)
        self.dense = nn.Dense(vocab_size, flatten=False)

    def init_state(self, enc_outputs, *args):
        return enc_outputs[1]

    def forward(self, X, state):
        X = self.embedding(X).swapaxes(0, 1)
        out, state = self.rnn(X, state)
        # Make the batch to be the first dimension to simplify loss computation.
```

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```
out = self.dense(out).swapaxes(0, 1)
return out, state
```

We create an decoder with the same hyper-parameters as the encoder. As can be seen, the output shape is changed to (batch size, the sequence length, vocabulary size).

```
decoder = Seq2SeqDecoder(vocab_size=10, embed_size=8,
                           num_hiddens=16, num_layers=2)
decoder.initialize()
state = decoder.init_state(encoder(X))
out, state = decoder(X, state)
out.shape, len(state), state[0].shape, state[1].shape
```

```
((4, 7, 10), 2, (2, 4, 16), (2, 4, 16))
```

### 10.14.3 The Loss Function

For each time step, the decoder outputs a vocabulary size confident score vector to predict words. Similar to language modeling, we can apply softmax to obtain the probabilities and then use cross-entropy loss to calculate the loss. But note that we padded the target sentences to make them have the same length. We would not like to compute the loss on the padding symbols.

To implement the loss function that filters out some entries, we will use an operator called `SequenceMask`. It can specify to mask the first dimension (`axis=0`) or the second one (`axis=1`). If the second one is chosen, given a valid length vector `len` and 2-dim input `X`, this operator sets `X[i, len[i]:] = 0` for all  $i$ 's.

```
X = nd.array([[1,2,3], [4,5,6]])
nd.SequenceMask(X, nd.array([1,2]), True, axis=1)
```

```
[[1. 0. 0.]
 [4. 5. 0.]]
<NDArray 2x3 @cpu(0)>
```

Apply to  $n$ -dim tensor  $X$ , it sets  $X[i, len[i]:, :, \dots, :] = 0$ . In addition, we can specify the filling value beyond 0.

```
X = nd.ones((2, 3, 4))
nd.SequenceMask(X, nd.array([1,2]), True, value=-1, axis=1)
```

```
[[[ 1.  1.  1.  1.]
  [-1. -1. -1. -1.]
  [-1. -1. -1. -1.]]

 [[ 1.  1.  1.  1.]
  [ 1.  1.  1.  1.]
  [-1. -1. -1. -1.]]]
<NDArray 2x3x4 @cpu(0)>
```

Now we can implement the masked version of the softmax cross-entropy loss. Note that each Gluon loss function allows to specify per-example weights, in default they are 1s. Then we can just use a zero weight for each example we would like to remove. So our customized loss function accepts an additional `valid_length` argument to ignore some failing elements in each sequence.

```
# Save to the d2l package.
class MaskedSoftmaxCELoss(gluon.loss.SoftmaxCELoss):
    # pred shape: (batch_size, seq_len, vocab_size)
    # label shape: (batch_size, seq_len)
    # valid_length shape: (batch_size, )
    def forward(self, pred, label, valid_length):
        # the sample weights shape should be (batch_size, seq_len, 1)
        weights = nd.ones_like(label).expand_dims(axis=-1)
        weights = nd.SequenceMask(weights, valid_length, True, axis=1)
        return super(MaskedSoftmaxCELoss, self).forward(pred, label, weights)
```

For a sanity check, we create identical three sequences, keep 4 elements for the first sequence, 2 elements for the second sequence, and none for the last one. Then the first example loss should be 2 times larger than the second one, and the last loss should be 0.

```
loss = MaskedSoftmaxCELoss()
loss(nd.ones((3, 4, 10)), nd.ones((3, 4)), nd.array([4, 2, 0]))
```

```
[2.3025851 1.1512926 0.]
<NDArray 3 @cpu(0)>
```

## 10.14.4 Training

During training, if the target sequence has length  $n$ , we feed the first  $n - 1$  tokens into the decoder as inputs, and the last  $n - 1$  tokens are used as ground truth label.

```
# Save to the d2l package.
def train_s2s_ch8(model, data_iter, lr, num_epochs, ctx):
    model.initialize(init.Xavier(), force_reinit=True, ctx=ctx)
    trainer = gluon.Trainer(model.collect_params(),
                            'adam', {'learning_rate': lr})
    loss = MaskedSoftmaxCELoss()
    #tic = time.time()
    animator = d2l.Animator(xlabel='epoch', ylabel='loss',
                             xlim=[1, num_epochs], ylim=[0, 0.25])
    for epoch in range(1, num_epochs+1):
        timer = d2l.Timer()
        metric = d2l.Accumulator(2) # loss_sum, num_tokens
        for batch in data_iter:
            X, X_vlen, Y, Y_vlen = [x.as_in_context(ctx) for x in batch]
            Y_input, Y_label, Y_vlen = Y[:, :-1], Y[:, 1:], Y_vlen-1
            with autograd.record():
                Y_hat, _ = model(X, Y_input, X_vlen, Y_vlen)
                l = loss(Y_hat, Y_label, Y_vlen)
            l.backward()
            d2l.grad_clipping(model, 1)
            num_tokens = Y_vlen.sum().asscalar()
            trainer.step(num_tokens)
            metric.add(l.sum().asscalar(), num_tokens)
        if epoch % 10 == 0:
            animator.add(epoch, metric[0]/metric[1])
```

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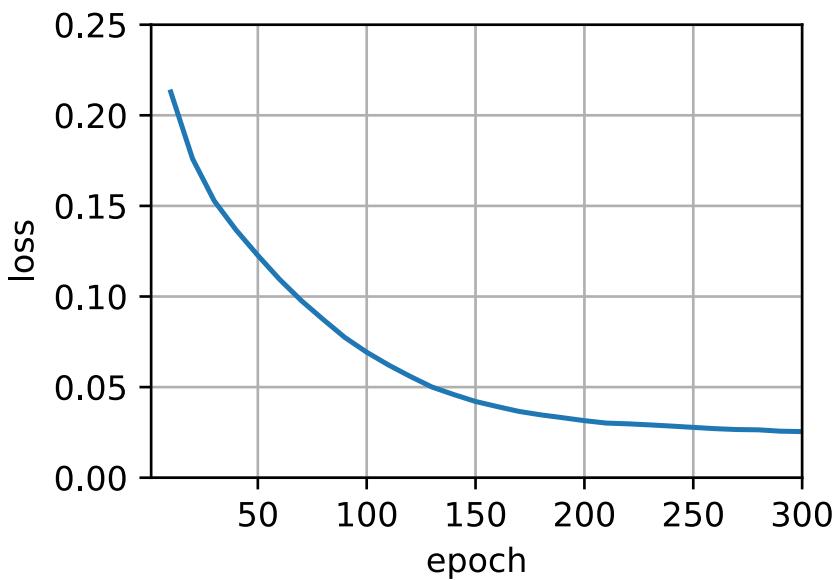
```
print('loss %.3f, %d tokens/sec on %s' % (
    metric[0]/metric[1], metric[1]/timer.stop(), ctx))
```

Next, we create a model instance and set hyper-parameters. Then, we can train the model.

```
embed_size, num_hiddens, num_layers, dropout = 32, 32, 2, 0.0
batch_size, num_steps = 64, 10
lr, num_epochs, ctx = 0.005, 300, d2l.try_gpu()

src_vocab, tgt_vocab, train_iter = d2l.load_data_nmt(batch_size, num_steps)
encoder = Seq2SeqEncoder(
    len(src_vocab), embed_size, num_hiddens, num_layers, dropout)
decoder = Seq2SeqDecoder(
    len(tgt_vocab), embed_size, num_hiddens, num_layers, dropout)
model = d2l.EncoderDecoder(encoder, decoder)
train_s2s_ch8(model, train_iter, lr, num_epochs, ctx)
```

```
loss 0.025, 10757 tokens/sec on gpu(0)
```



### 10.14.5 Predicting

Here we implement the simplest method, greedy search, to generate an output sequence. During predicting, we feed the same “<bos>” token to the decoder as training at time step 0. But the input token for a later time step is the predicted token from the previous time step.

```
# Save to the d2l package.
def predict_s2s_ch8(model, src_sentence, src_vocab, tgt_vocab, num_steps, ctx):
    src_tokens = src_vocab[src_sentence.lower().split(' ')]
    enc_valid_length = nd.array([len(src_tokens)], ctx=ctx)
    src_tokens = d2l.trim_pad(src_tokens, num_steps, src_vocab.pad)
    enc_X = nd.array(src_tokens, ctx=ctx)
```

(continues on next page)

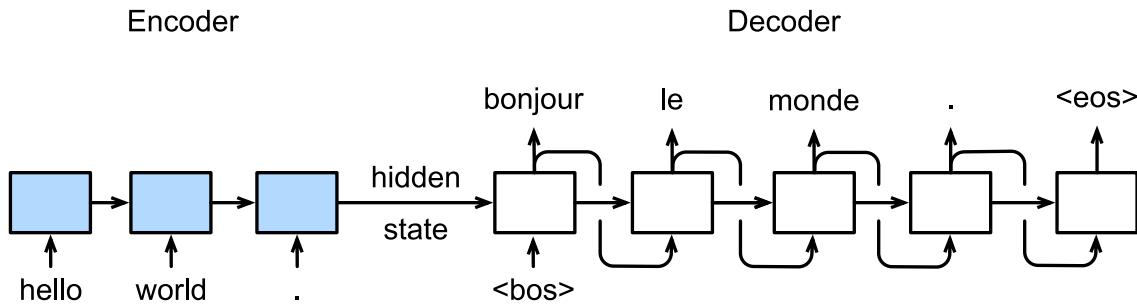


Fig. 10.14.2: Sequence to sequence model predicting with greedy search

(continued from previous page)

```
# add the batch_size dimension.
enc_outputs = model.encoder(enc_X.expand_dims(axis=0), enc_valid_length)
dec_state = model.decoder.init_state(enc_outputs, enc_valid_length)
dec_X = nd.array([tgt_vocab.bos], ctx=ctx).expand_dims(axis=0)
predict_tokens = []
for _ in range(num_steps):
    Y, dec_state = model.decoder(dec_X, dec_state)
    # The token with highest score is used as the next time step input.
    dec_X = Y.argmax(axis=2)
    py = dec_X.squeeze(axis=0).astype('int32').asscalar()
    if py == tgt_vocab.eos:
        break
    predict_tokens.append(py)
return ' '.join(tgt_vocab.to_tokens(predict_tokens))
```

Try several examples:

```
for sentence in ['Go .', 'Wow !', "I'm OK .", 'I won !']:
    print(sentence + ' => ' + predict_s2s_ch8(
        model, sentence, src_vocab, tgt_vocab, num_steps, ctx))
```

```
Go . => va !
Wow ! => <unk> !
I'm OK . => je vais bien .
I won ! => je l'ai emporté !
```

## 10.14.6 Summary

## 10.15 Beam Search

In Section 10.14, we discussed how to train an encoder-decoder with input and output sequences that are both of variable length. In this section, we are going to introduce how to use the encoder-decoder to predict sequences of variable length.

As in the previous section, when preparing to train the data set, we normally attach a special symbol “<eos>” after each sentence to indicate the termination of the sequence. We will continue to use this mathematical symbol in the discussion below. For ease of discussion, we assume that the output of the decoder is a sequence

of text. Let the size of output text dictionary  $\mathcal{Y}$  (contains special symbol “<eos>”) be  $|\mathcal{Y}|$ , and the maximum length of the output sequence be  $T'$ . There are a total  $\mathcal{O}(|\mathcal{Y}|^{T'})$  types of possible output sequences. All the subsequences after the special symbol “<eos>” in these output sequences will be discarded.

### 10.15.1 Greedy Search

First, we will take a look at a simple solution: greedy search. For any time step  $t'$  of the output sequence, we are going to search for the word with the highest conditional probability from  $|\mathcal{Y}|$  numbers of words, with

$$y_{t'} = \underset{y \in \mathcal{Y}}{\operatorname{argmax}} \mathbb{P}(y \mid y_1, \dots, y_{t'-1}, \mathbf{c}) \quad (10.15.1)$$

as the output. Once the “<eos>” symbol is detected, or the output sequence has reached its maximum length  $T'$ , the output is completed.

As we mentioned in our discussion of the decoder, the conditional probability of generating an output sequence based on the input sequence is  $\prod_{t'=1}^{T'} \mathbb{P}(y_{t'} \mid y_1, \dots, y_{t'-1}, \mathbf{c})$ . We will take the output sequence with the highest conditional probability as the optimal sequence. The main problem with greedy search is that there is no guarantee that the optimal sequence will be obtained.

Take a look at the example below. We assume that there are four words “A”, “B”, “C”, and “<eos>” in the output dictionary. The four numbers under each time step in Fig. 10.15.1 represent the conditional probabilities of generating “A”, “B”, “C”, and “<eos>” at that time step. At each time step, greedy search selects the word with the highest conditional probability. Therefore, the output sequence “A”, “B”, “C”, “<eos>” will be generated in Fig. 10.15.1. The conditional probability of this output sequence is  $0.5 \times 0.4 \times 0.4 \times 0.6 = 0.048$ .

	Time step	1	2	3	4
A	0.5	0.1	0.2	0.0	
B	0.2	0.4	0.2	0.2	
C	0.2	0.3	0.4	0.2	
<eos>	0.1	0.2	0.2	0.6	

Fig. 10.15.1: The four numbers under each time step represent the conditional probabilities of generating “A”, “B”, “C”, and “<eos>” at that time step. At each time step, greedy search selects the word with the highest conditional probability.

Now, we will look at another example shown in Fig. 10.15.2. Unlike in Fig. 10.15.1, Fig. 10.15.2 selects the word “C” for it has the second highest conditional probability at time step 2. Since the output subsequences of time steps 1 and 2, on which time step 3 is based, are changed from “A” and “B” in Fig. 10.15.1 to “A” and “C” in Fig. 10.15.2, the conditional probability of each word generated at time step 3 has also changed in Fig. 10.15.2. We choose the word “B”, which has the highest conditional probability. Now, the output subsequences of time step 4 based on the first three time steps are “A”, “C”, and “B”, which are different from “A”, “B”, and “C” in Fig. 10.15.1. Therefore, the conditional probability of generating each word in time step 4 in Fig. 10.15.2 is also different from that in Fig. 10.15.1. We find that the conditional probability of the output sequence “A”, “C”, “B”, “<eos>” at the current time step is  $0.5 \times 0.3 \times 0.6 \times 0.6 = 0.054$ , which is higher than the conditional probability of the output sequence obtained by greedy search. Therefore, the output sequence “A”, “B”, “C”, “<eos>” obtained by the greedy search is not an optimal sequence.

	Time step	1	2	3	4
A	0.5	0.1	0.1	0.1	
B	0.2	0.4	0.6	0.2	
C	0.2	0.3	0.2	0.1	
<eos>	0.1	0.2	0.1	0.6	

Fig. 10.15.2: The four numbers under each time step represent the conditional probabilities of generating “A”, “B”, “C”, and “<eos>” at that time step. At time step 2, the word “C”, which has the second highest conditional probability, is selected.

### 10.15.2 Exhaustive Search

If the goal is to obtain the optimal sequence, we may consider using exhaustive search: an exhaustive examination of all possible output sequences, which outputs the sequence with the highest conditional probability.

Although we can use an exhaustive search to obtain the optimal sequence, its computational overhead  $\mathcal{O}(|\mathcal{Y}|^{T'})$  is likely to be excessively high. For example, when  $|\mathcal{Y}| = 10000$  and  $T' = 10$ , we will need to evaluate  $10000^{10} = 10^{40}$  sequences. This is next to impossible to complete. The computational overhead of greedy search is  $\mathcal{O}(|\mathcal{Y}| T')$ , which is usually significantly less than the computational overhead of an exhaustive search. For example, when  $|\mathcal{Y}| = 10000$  and  $T' = 10$ , we only need to evaluate  $10000 \times 10 = 1 \times 10^5$  sequences.

### 10.15.3 Beam Search

Beam search is an improved algorithm based on greedy search. It has a hyper-parameter named beam size. We set it to  $k$ . At time step 1, we select  $k$  words with the highest conditional probability to be the first words of the  $k$  candidate output sequences. For each subsequent time step, we are going to select the  $k$  output sequences with the highest conditional probability from the total of  $k |\mathcal{Y}|$  possible output sequences based on the  $k$  candidate output sequences from the previous time step. These will be the candidate output sequence for that time step. Finally, we will filter out the sequences containing the special symbol “<eos>” from the candidate output sequences of each time step and discard all the subsequences after it to obtain a set of final candidate output sequences.

Fig. 10.15.3 demonstrates the process of beam search with an example. Suppose that the vocabulary of the output sequence only contains five elements:  $\mathcal{Y} = \{A, B, C, D, E\}$  where one of them is a special symbol “<eos>”. Set beam size to 2, the maximum length of the output sequence to 3. At time step 1 of the output sequence, suppose the words with the highest conditional probability  $\mathbb{P}(y_1 | \mathbf{c})$  are  $A$  and  $C$ . At time step 2, we compute  $\mathbb{P}(A, y_2 | \mathbf{c}) = \mathbb{P}(A | \mathbf{c})\mathbb{P}(y_2 | A, \mathbf{c})$  and  $\mathbb{P}(C, y_2 | \mathbf{c}) = \mathbb{P}(C | \mathbf{c})\mathbb{P}(y_2 | C, \mathbf{c})$  for all  $y_2 \in \mathcal{Y}$ , and pick the largest two among these 10 values: say  $\mathbb{P}(A, B | \mathbf{c})$  and  $\mathbb{P}(C, E | \mathbf{c})$ . Then at time step 3, we compute  $\mathbb{P}(A, B, y_3 | \mathbf{c}) = \mathbb{P}(A, B | \mathbf{c})\mathbb{P}(y_3 | A, B, \mathbf{c})$  and  $\mathbb{P}(C, E, y_3 | \mathbf{c}) = \mathbb{P}(C, E | \mathbf{c})\mathbb{P}(y_3 | C, E, \mathbf{c})$  for all  $y_3 \in \mathcal{Y}$ , and pick the largest two among these 10 values: say  $\mathbb{P}(A, B, D | \mathbf{c})$  and  $\mathbb{P}(C, E, D | \mathbf{c})$ . As a result, we obtain 6 candidates output sequences: (1)  $A$ ; (2)  $C$ ; (3)  $A, B$ ; (4)  $C, E$ ; (5)  $A, B, D$ ; and (6)  $C, E, D$ . In the end, we will get the set of final candidate output sequences based on these 6 sequences.

In the set of final candidate output sequences, we will take the sequence with the highest score as the output sequence from those below:

$$\frac{1}{L^\alpha} \log \mathbb{P}(y_1, \dots, y_L) = \frac{1}{L^\alpha} \sum_{t'=1}^L \log \mathbb{P}(y_{t'} | y_1, \dots, y_{t'-1}, \mathbf{c}), \quad (10.15.2)$$

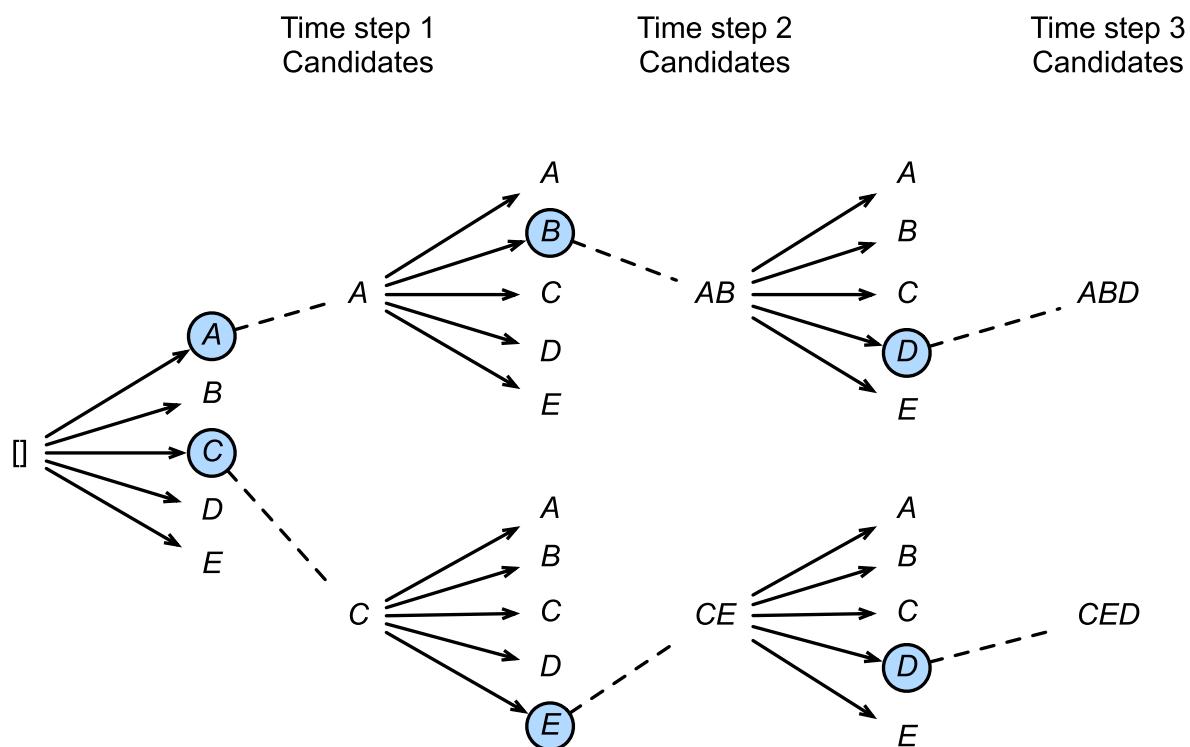


Fig. 10.15.3: The beam search process. The beam size is 2 and the maximum length of the output sequence is 3. The candidate output sequences are A, C, AB, CE, ABD, and CED.

Here,  $L$  is the length of the final candidate sequence and the selection for  $\alpha$  is generally 0.75. The  $L^\alpha$  on the denominator is a penalty on the logarithmic addition scores for the longer sequences above. The computational overhead  $\mathcal{O}(k|\mathcal{Y}|T')$  of the beam search can be obtained through analysis. The result is a computational overhead between those of greedy search and exhaustive search. In addition, greedy search can be treated as a beam search with a beam size of 1. Beam search strikes a balance between computational overhead and search quality using a flexible beam size of  $k$ .

#### 10.15.4 Summary

- Methods for predicting variable-length sequences include greedy search, exhaustive search, and beam search.
- Beam search strikes a balance between computational overhead and search quality using a flexible beam size.

#### 10.15.5 Exercises

- Can we treat an exhaustive search as a beam search with a special beam size? Why?
- We used language models to generate sentences in [Section 10.5](#). Which kind of search does this output use? Can you improve it?

#### 10.15.6 Scan the QR Code to Discuss<sup>157</sup>



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<sup>157</sup> <https://discuss.mxnet.io/t/2394>



## ATTENTION MECHANISM

Attention is a generalized pooling method with bias alignment over inputs.

### 11.1 Attention Mechanism

In Section 10.14, we encode the source sequence input information in the recurrent unit state and then pass it to the decoder to generate the target sequence. A token in the target sequence may closely relate to some tokens in the source sequence instead of the whole source sequence. For example, when translating “Hello world.” to “Bonjour le monde.”, “Bonjour” maps to “Hello” and “monde” maps to “world”. In the seq2seq model, the decoder may implicitly select the corresponding information from the state passed by the decoder. The attention mechanism, however, makes this selection explicit.

Attention is a generalized pooling method with bias alignment over inputs. The core component in the attention mechanism is the attention layer, or called attention for simplicity. An input of the attention layer is called a query. For a query, the attention layer returns the output based on its memory, which is a set of key-value pairs. To be more specific, assume a query  $\mathbf{q} \in \mathbb{R}^{d_q}$ , and the memory contains  $n$  key-value pairs,  $(\mathbf{k}_1, \mathbf{v}_1), \dots, (\mathbf{k}_n, \mathbf{v}_n)$ , with  $\mathbf{k}_i \in \mathbb{R}^{d_k}$ ,  $\mathbf{v}_i \in \mathbb{R}^{d_v}$ . The attention layer then returns an output  $\mathbf{o} \in \mathbb{R}^{d_v}$  with the same shape as a value.

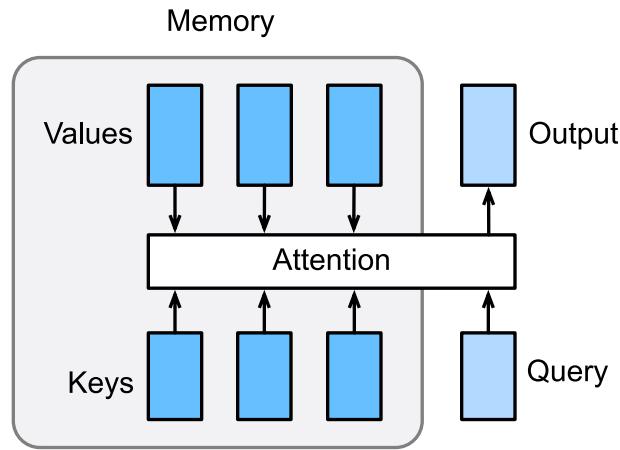


Fig. 11.1.1: The attention layer returns an output based on the input query and its memory.

To compute the output, we first assume there is a score function  $\alpha$  which measures the similarity between the query and a key. Then we compute all  $n$  scores  $a_1, \dots, a_n$  by

$$a_i = \alpha(\mathbf{q}, \mathbf{k}_i). \quad (11.1.1)$$

Next we use softmax to obtain the attention weights

$$b_1, \dots, b_n = \text{softmax}(a_1, \dots, a_n). \quad (11.1.2)$$

The output is then a weighted sum of the values

$$\mathbf{o} = \sum_{i=1}^n b_i \mathbf{v}_i. \quad (11.1.3)$$

Different choices of the score function lead to different attention layers. We will discuss two commonly used attention layers in the rest of this section. Before diving into the implementation, we first introduce a masked version of the softmax operator and explain a specialized dot operator `nd.batched_dot`.

```
import math
from mxnet import nd
from mxnet.gluon import nn
```

The masked softmax takes a 3-dim input and allows us to filter out some elements by specifying valid lengths for the last dimension. (Refer to [Section 10.12](#) for the definition of a valid length.)

```
# Save to the d2l package.
def masked_softmax(X, valid_length):
    # X: 3-D tensor, valid_length: 1-D or 2-D tensor
    if valid_length is None:
        return X.softmax()
    else:
        shape = X.shape
        if valid_length.ndim == 1:
            valid_length = valid_length.repeat(shape[1], axis=0)
        else:
            valid_length = valid_length.reshape((-1,))
        # fill masked elements with a large negative, whose exp is 0
        X = nd.SequenceMask(X.reshape((-1, shape[-1])), valid_length, True,
                            axis=1, value=-1e6)
    return X.softmax().reshape(shape)
```

Construct two examples, where each example is a 2-by-4 matrix, as the input. If we specify the valid length for the first example to be 2, then only the first two columns of this example are used to compute softmax.

```
masked_softmax(nd.random.uniform(shape=(2, 2, 4)), nd.array([2, 3]))
```

```
[[[0.488994  0.511006  0.        ]
 [0.43654838 0.56345165 0.        ]]
 [[0.28817102 0.3519408  0.3598882  0.
 [0.29034293 0.25239873 0.45725834 0.        ]]
 <NDArray 2x2x4 @cpu(0)>
```

The operator `nd.batched_dot` takes two inputs  $X$  and  $Y$  with shapes  $(b, n, m)$  and  $(b, m, k)$ , respectively. It computes  $b$  dot products, with  $Z[i,:,:] = \text{dot}(X[i,:,:], Y[i,:,:])$  for  $i = 1, \dots, n$ .

```
nd.batch_dot(nd.ones((2, 1, 3)), nd.ones((2, 3, 2)))
```

```
[[[3. 3.]]
 [[3. 3.]]]
<NDArray 2x1x2 @cpu(0)>
```

### 11.1.1 Dot Product Attention

The dot product assumes the query has the same dimension as the keys, namely  $\mathbf{q}, \mathbf{k}_i \in \mathbb{R}^d$  for all  $i$ . It computes the score by an inner product between the query and a key, often then divided by  $\sqrt{d}$  to make the scores less sensitive to the dimension  $d$ . In other words,

$$\alpha(\mathbf{q}, \mathbf{k}) = \langle \mathbf{q}, \mathbf{k} \rangle / \sqrt{d}. \quad (11.1.4)$$

Assume  $\mathbf{Q} \in \mathbb{R}^{m \times d}$  contains  $m$  queries and  $\mathbf{K} \in \mathbb{R}^{n \times d}$  has all  $n$  keys. We can compute all  $mn$  scores by

$$\alpha(\mathbf{Q}, \mathbf{K}) = \mathbf{Q}\mathbf{K}^T / \sqrt{d}. \quad (11.1.5)$$

Now let's implement this layer that supports a batch of queries and key-value pairs. In addition, it supports randomly dropping some attention weights as a regularization.

```
# Save to the d2l package.
class DotProductAttention(nn.Block):
    def __init__(self, dropout, **kwargs):
        super(DotProductAttention, self).__init__(**kwargs)
        self.dropout = nn.Dropout(dropout)

    # query: (batch_size, #queries, d)
    # key: (batch_size, #kv_pairs, d)
    # value: (batch_size, #kv_pairs, dim_v)
    # valid_length: either (batch_size, ) or (batch_size, xx)
    def forward(self, query, key, value, valid_length=None):
        d = query.shape[-1]
        # set transpose_b=True to swap the last two dimensions of key
        scores = nd.batch_dot(query, key, transpose_b=True) / math.sqrt(d)
        attention_weights = self.dropout(nd.softmax(scores, valid_length))
        return nd.batch_dot(attention_weights, value)
```

Now we create two batches, and each batch has one query and 10 key-value pairs. We specify through `valid_length` that for the first batch, we will only pay attention to the first 2 key-value pairs, while for the second batch, we will check the first 6 key-value pairs. Therefore, though both batches have the same query and key-value pairs, we obtain different outputs.

```
atten = DotProductAttention(dropout=0.5)
atten.initialize()
keys = nd.ones((2, 10, 2))
values = nd.arange(40).reshape((1, 10, 4)).repeat(2, axis=0)
atten(nd.ones((2, 1, 2)), keys, values, nd.array([2, 6]))
```

```
[[[ 2.       3.       4.       5.       ]]
 [[10.       11.       12.000001 13.       ]]]
<NDArray 2x1x4 @cpu(0)>
```

### 11.1.2 Multilayer Perceptron Attention

In multilayer perceptron attention, we first project both query and keys into  $\mathbb{R}^h$ .

To be more specific, assume learnable parameters  $\mathbf{W}_k \in \mathbb{R}^{h \times d_k}$ ,  $\mathbf{W}_q \in \mathbb{R}^{h \times d_q}$ , and  $\mathbf{v} \in \mathbb{R}^p$ . Then the score function is defined by

$$\alpha(\mathbf{k}, \mathbf{q}) = \mathbf{v}^T \tanh(\mathbf{W}_k \mathbf{k} + \mathbf{W}_q \mathbf{q}). \quad (11.1.6)$$

This concatenates the key and value in the feature dimension and feeds them into a single hidden layer perceptron with hidden layer size  $h$  and output layer size 1. The hidden layer activation function is tanh and no bias is applied.

```
# Save to the d2l package.
class MLPAttention(nn.Block):
    def __init__(self, units, dropout, **kwargs):
        super(MLPAttention, self).__init__(**kwargs)
        # Use flatten=True to keep query's and key's 3-D shapes.
        self.W_k = nn.Dense(units, activation='tanh',
                            use_bias=False, flatten=False)
        self.W_q = nn.Dense(units, activation='tanh',
                            use_bias=False, flatten=False)
        self.v = nn.Dense(1, use_bias=False, flatten=False)
        self.dropout = nn.Dropout(dropout)

    def forward(self, query, key, value, valid_length):
        query, key = self.W_k(query), self.W_q(key)
        # expand query to (batch_size, #querys, 1, units), and key to
        # (batch_size, 1, #kv_pairs, units). Then plus them with broadcast.
        features = query.expand_dims(axis=2) + key.expand_dims(axis=1)
        scores = self.v(features).squeeze(axis=-1)
        attention_weights = self.dropout(masked_softmax(scores, valid_length))
        return nd.batch_dot(attention_weights, value)
```

Despite MLPAttention containing an additional MLP model, given the same inputs with identical keys, we obtain the same output as for DotProductAttention.

```
atten = MLPAttention(units=8, dropout=0.1)
atten.initialize()
atten(nd.ones((2,1,2)), keys, values, nd.array([2, 6]))
```

```
[[[ 2.       3.       4.       5.       ]]

 [[10.       11.       12.000001 13.       ]]]
<NDArray 2x1x4 @cpu(0)>
```

### 11.1.3 Summary

- An attention layer explicitly selects related information.
- An attention layer's memory consists of key-value pairs, so its output is close to the values whose keys are similar to the query.

## 11.2 Sequence to Sequence with Attention Mechanism

In this section, we add the attention mechanism to the sequence to sequence model introduced in Section 10.14 to explicitly select state. Fig. 11.2.1 shows the model architecture for a decoding time step. As can be seen, the memory of the attention layer consists of the encoder outputs of each time step. During decoding, the decoder output from the previous time step is used as the query, the attention output is then fed into the decoder with the input to provide attentional context information.

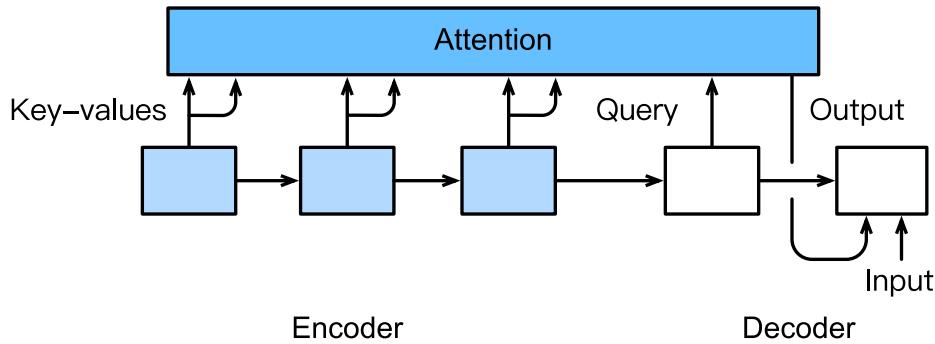


Fig. 11.2.1: The second time step in decoding for the sequence to sequence model with attention mechanism.

The layer structure in the encoder and the decoder is shown in Fig. 11.2.2.

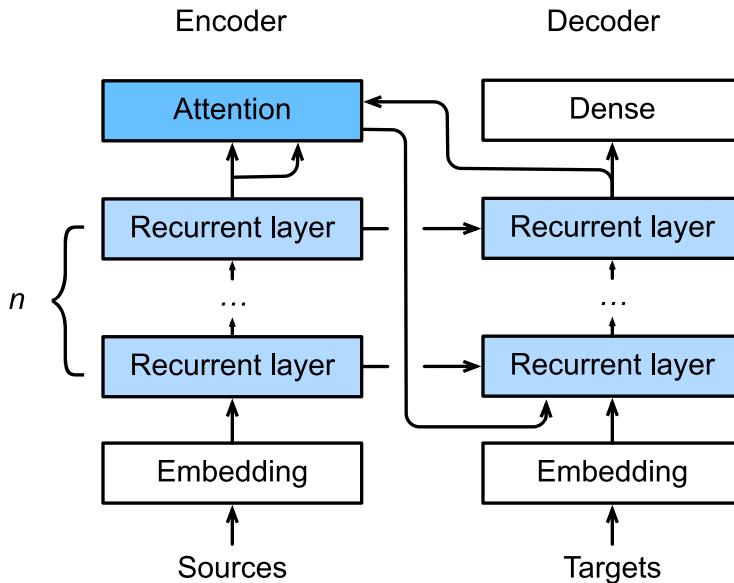


Fig. 11.2.2: The layers in the sequence to sequence model with attention mechanism.

```
import d2l
from mxnet import nd
from mxnet.gluon import rnn, nn
```

### 11.2.1 Decoder

Now let's implement the decoder of this model. We add a MLP attention layer which has the same hidden size as the LSTM layer. The state passed from the encoder to the decoder contains three items:

- the encoder outputs of all time steps, which are used as the attention layer's memory with identical keys and values
- the hidden state of the last time step that is used to initialize the encoder's hidden state
- valid lengths of the decoder inputs so the attention layer will not consider encoder outputs for padding tokens.

In each time step of decoding, we use the output of the last RNN layer as the query for the attention layer. Its output is then concatenated with the input embedding vector to feed into the RNN layer. Despite the RNN layer hidden state also contains history information from decoder, the attention output explicitly selects the encoder outputs that are correlated to the query and suspends other non-correlated information.

```
class Seq2SeqAttentionDecoder(d2l.Decoder):
    def __init__(self, vocab_size, embed_size, num_hiddens, num_layers,
                 dropout=0, **kwargs):
        super(Seq2SeqAttentionDecoder, self).__init__(**kwargs)
        self.attention_cell = d2l.MLPAttention(num_hiddens, dropout)
        self.embedding = nn.Embedding(vocab_size, embed_size)
        self.rnn = rnn.LSTM(num_hiddens, num_layers, dropout=dropout)
        self.dense = nn.Dense(vocab_size, flatten=False)

    def init_state(self, enc_outputs, enc_valid_len, *args):
        outputs, hidden_state = enc_outputs
        # Transpose outputs to (batch_size, seq_len, hidden_size)
        return (outputs.swapaxes(0, 1), hidden_state, enc_valid_len)

    def forward(self, X, state):
        enc_outputs, hidden_state, enc_valid_len = state
        X = self.embedding(X).swapaxes(0, 1)
        outputs = []
        for x in X:
            # query shape: (batch_size, 1, hidden_size)
            query = hidden_state[0][-1].expand_dims(axis=1)
            # context has same shape as query
            context = self.attention_cell(
                query, enc_outputs, enc_outputs, enc_valid_len)
            # concatenate on the feature dimension
            x = nd.concat(context, x.expand_dims(axis=1), dim=-1)
            # reshape x to (1, batch_size, embed_size+hidden_size)
            out, hidden_state = self.rnn(x.swapaxes(0, 1), hidden_state)
            outputs.append(out)
        outputs = self.dense(nd.concat(*outputs, dim=0))
        return outputs.swapaxes(0, 1), [enc_outputs, hidden_state,
                                         enc_valid_len]
```

Use the same hyper-parameters to create an encoder and decoder as in Section 10.14, we get the same decoder output shape, but the state structure is changed.

```

encoder = d2l.Seq2SeqEncoder(vocab_size=10, embed_size=8,
                               num_hiddens=16, num_layers=2)
encoder.initialize()
decoder = Seq2SeqAttentionDecoder(vocab_size=10, embed_size=8,
                                   num_hiddens=16, num_layers=2)
decoder.initialize()
X = nd.zeros((4, 7))
state = decoder.init_state(encoder(X), None)
out, state = decoder(X, state)
out.shape, len(state), state[0].shape, len(state[1]), state[1][0].shape

```

```
((4, 7, 10), 3, (4, 7, 16), 2, (2, 4, 16))
```

## 11.2.2 Training

Again, we use the same training hyper-parameters as in Section 10.14. The training loss is similar to the seq2seq model, because the sequences in the training dataset are relative short. The additional attention layer doesn't lead to a significant different. But due to both attention layer computational overhead and we unroll the time steps in the decoder, this model is much slower than the seq2seq model.

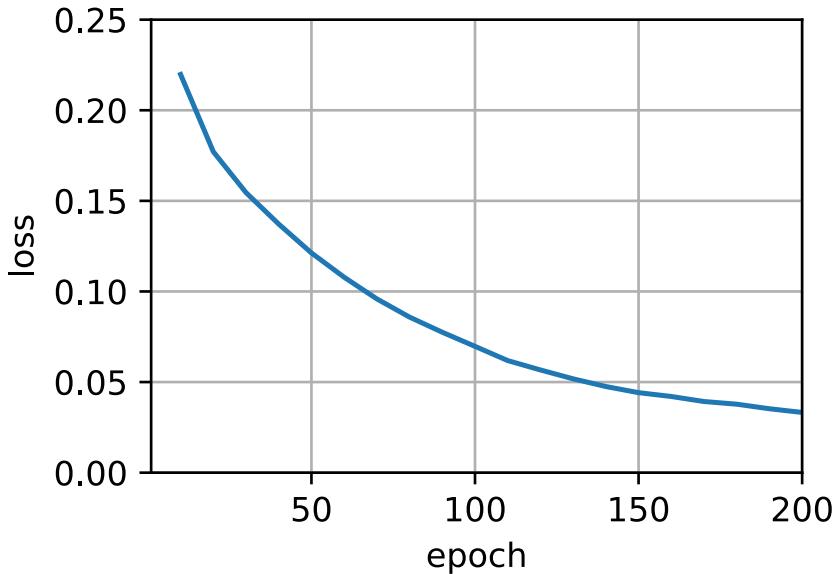
```

embed_size, num_hiddens, num_layers, dropout = 32, 32, 2, 0.0
batch_size, num_steps = 64, 10
lr, num_epochs, ctx = 0.005, 200, d2l.try_gpu()

src_vocab, tgt_vocab, train_iter = d2l.load_data_nmt(batch_size, num_steps)
encoder = d2l.Seq2SeqEncoder(
    len(src_vocab), embed_size, num_hiddens, num_layers, dropout)
decoder = Seq2SeqAttentionDecoder(
    len(tgt_vocab), embed_size, num_hiddens, num_layers, dropout)
model = d2l.EncoderDecoder(encoder, decoder)
d2l.train_s2s_ch8(model, train_iter, lr, num_epochs, ctx)

```

```
loss 0.033, 4409 tokens/sec on gpu(0)
```



Lastly, we predict several sample examples.

```
for sentence in ['Go .', 'Wow !', "I'm OK .", 'I won !']:
    print(sentence + ' => ' + d2l.predict_s2s_ch8(
        model, sentence, src_vocab, tgt_vocab, num_steps, ctx))
```

```
Go . => va !
Wow ! => <unk> !
I'm OK . => je vais bien .
I won ! => je l'ai emporté !
```

### 11.2.3 Summary

- Seq2seq with attention adds an additional attention layer to use encoder's outputs as memory and its output is used as part of decoder's input.

## 11.3 Transformer

The Transformer model is also based on the encoder-decoder architecture. It, however, differs to the seq2seq model that the transformer replaces the recurrent layers in seq2seq with attention layers. To deal with sequential inputs, each item in the sequential is copied as the query, the key and the value as illustrated in Fig. 11.3.1. It therefore outputs a same length sequential output. We call such an attention layer as a self-attention layer.

The transformer architecture, with a comparison to the seq2seq model with attention, is shown in Fig. 11.3.2. These two models are similar to each other in overall: the source sequence embeddings are fed into  $n$  repeated blocks. The outputs of the last block are then used as attention memory for the decoder. The target sequence embeddings are similarly fed into  $n$  repeated blocks in the decoder, and the final outputs are obtained by applying a dense layer with vocabulary size to the last block's outputs.

It can also be seen that the transformer differs to the seq2seq with attention model in three major places:

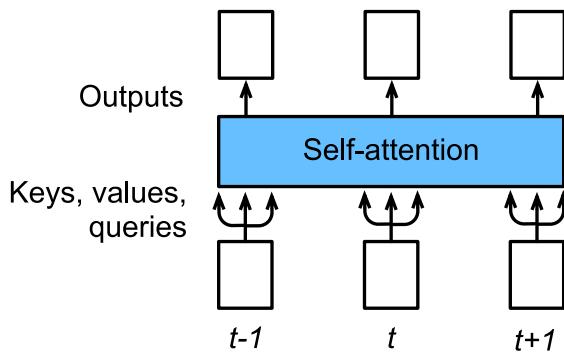


Fig. 11.3.1: Self-attention architecture.

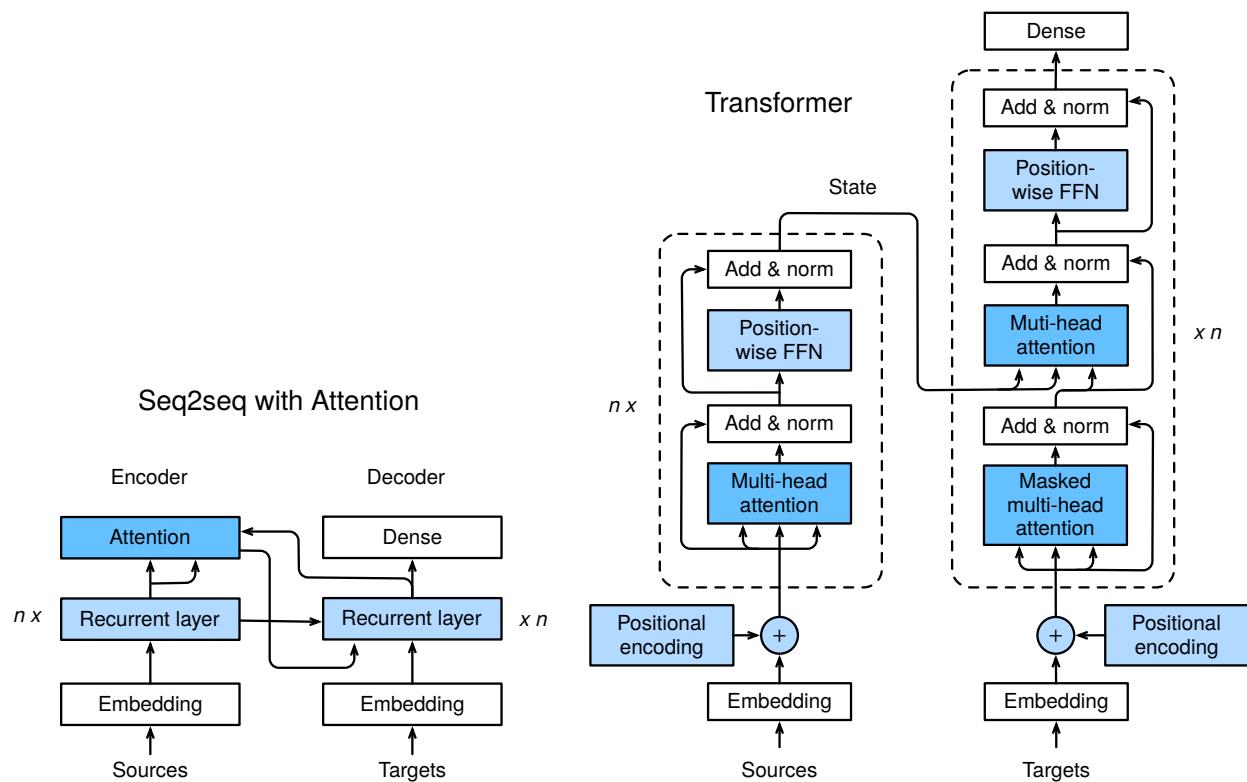


Fig. 11.3.2: The transformer architecture.

1. A recurrent layer in seq2seq is replaced with a transformer block. This block contains a self-attention layer (multi-head attention) and a network with two dense layers (position-wise FFN) for the encoder. For the decoder, another multi-head attention layer is used to take the encoder state.
2. The encoder state is passed to every transformer block in the decoder, instead of using as an additional input of the first recurrent layer in seq2seq.
3. Since the self-attention layer does not distinguish the item order in a sequence, a positional encoding layer is used to add sequential information into each sequence item.

In the rest of this section, we will explain every new layer introduced by the transformer, and construct a model to train on the machine translation dataset.

```
import math
import d2l
from mxnet import nd, autograd
from mxnet.gluon import nn
```

### 11.3.1 Multi-Head Attention

A multi-head attention layer consists of  $h$  parallel attention layers, each one is called a head. For each head, we use three dense layers with hidden sizes  $p_q$ ,  $p_k$  and  $p_v$  to project the queries, keys and values, respectively, before feeding into the attention layer. The outputs of these  $h$  heads are concatenated and then projected by another dense layer.

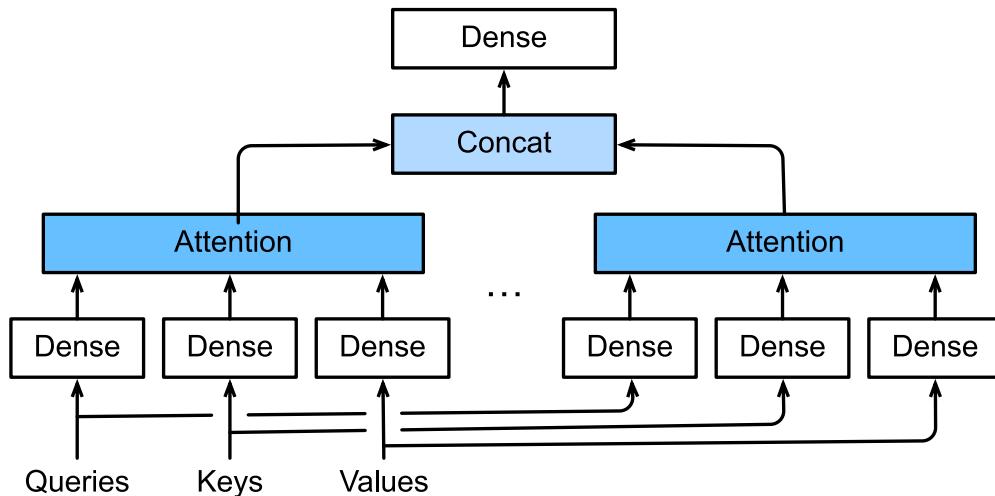


Fig. 11.3.3: Multi-head attention

To be more specific, assume we have the learnable parameters  $\mathbf{W}_q^{(i)} \in \mathbb{R}^{p_q \times d_q}$ ,  $\mathbf{W}_k^{(i)} \in \mathbb{R}^{p_k \times d_k}$ , and  $\mathbf{W}_v^{(i)} \in \mathbb{R}^{p_v \times d_v}$ , for  $i = 1, \dots, h$ , and  $\mathbf{W}_o \in \mathbb{R}^{d_o \times hp_v}$ . Then the output for each head can be obtained by

$$\mathbf{o}^{(i)} = \text{attention}(\mathbf{W}_q^{(i)} \mathbf{q}, \mathbf{W}_k^{(i)} \mathbf{k}, \mathbf{W}_v^{(i)} \mathbf{v}), \quad (11.3.1)$$

where attention can be any attention layer introduced before. Since we already have learnable parameters, the simple dot product attention is used.

Then we concatenate all outputs and project them to obtain the multi-head attention output

$$\mathbf{o} = \mathbf{W}_o \begin{bmatrix} \mathbf{o}^{(1)} \\ \vdots \\ \mathbf{o}^{(h)} \end{bmatrix}. \quad (11.3.2)$$

In practice, we often use  $p_q = p_k = p_v = d_o/h$ . The hyper-parameters for a multi-head attention, therefore, contain the number heads  $h$ , and output feature size  $d_o$ .

```
class MultiHeadAttention(nn.Block):
    def __init__(self, units, num_heads, dropout, **kwargs):  # units = d_o
        super(MultiHeadAttention, self).__init__(**kwargs)
        assert units % num_heads == 0
        self.num_heads = num_heads
        self.attention = d2l.DotProductAttention(dropout)
        self.W_q = nn.Dense(units, use_bias=False, flatten=False)
        self.W_k = nn.Dense(units, use_bias=False, flatten=False)
        self.W_v = nn.Dense(units, use_bias=False, flatten=False)

        # query, key, and value shape: (batch_size, num_items, dim)
        # valid_length shape is either (batch_size, ) or (batch_size, num_items)
    def forward(self, query, key, value, valid_length):
        # Project and transpose from (batch_size, num_items, units) to
        # (batch_size * num_heads, num_items, p), where units = p * num_heads.
        query, key, value = [transpose_qkv(X, self.num_heads) for X in (
            self.W_q(query), self.W_k(key), self.W_v(value))]
        if valid_length is not None:
            # Copy valid_length by num_heads times
            if valid_length.ndim == 1:
                valid_length = valid_length.tile(self.num_heads)
            else:
                valid_length = valid_length.tile((self.num_heads, 1))
        output = self.attention(query, key, value, valid_length)
        # Transpose from (batch_size * num_heads, num_items, p) back to
        # (batch_size, num_items, units)
        return transpose_output(output, self.num_heads)
```

Here are the definitions of the transpose functions.

```
def transpose_qkv(X, num_heads):
    # Shape after reshape: (batch_size, num_items, num_heads, p)
    # 0 means copying the shape element, -1 means inferring its value
    X = X.reshape((0, 0, num_heads, -1))
    # Swap the num_items and the num_heads dimensions
    X = X.transpose((0, 2, 1, 3))
    # Merge the first two dimensions. Use reverse=True to infer
    # shape from right to left
    return X.reshape((-1, 0, 0), reverse=True)

def transpose_output(X, num_heads):
    # A reversed version of transpose_qkv
    X = X.reshape((-1, num_heads, 0, 0), reverse=True)
    X = X.transpose((0, 2, 1, 3))
    return X.reshape((0, 0, -1))
```

Create a multi-head attention with the output size  $d_o$  equals to 100, the output will share the same batch size and sequence length as the input, but the last dimension will be equal to  $d_o$ .

```
cell = MultiHeadAttention(100, 10, 0.5)
cell.initialize()
X = nd.ones((2, 4, 5))
valid_length = nd.array([2,3])
cell(X, X, X, valid_length).shape
```

```
(2, 4, 100)
```

### 11.3.2 Position-wise Feed-Forward Networks

The position-wise feed-forward network accepts a 3-dim input with shape (batch size, sequence length, feature size). It consists of two dense layers that applies to the last dimension, which means the same dense layers are used for each position item in the sequence, so called position-wise.

```
class PositionWiseFFN(nn.Block):
    def __init__(self, units, hidden_size, **kwargs):
        super(PositionWiseFFN, self).__init__(**kwargs)
        self.ffn_1 = nn.Dense(hidden_size, flatten=False, activation='relu')
        self.ffn_2 = nn.Dense(units, flatten=False)

    def forward(self, X):
        return self.ffn_2(self.ffn_1(X))
```

Similar to the multi-head attention, the position-wise feed-forward network will only change the last dimension size of the input. In addition, if two items in the input sequence are identical, the according outputs will be identical as well.

```
ffn = PositionWiseFFN(4, 8)
ffn.initialize()
ffn(nd.ones((2, 3, 4)))[0]
```

```
[[ 0.00752072  0.00865059  0.01013744 -0.00906538]
 [ 0.00752072  0.00865059  0.01013744 -0.00906538]
 [ 0.00752072  0.00865059  0.01013744 -0.00906538]]
<NDArray 3x4 @cpu(0)>
```

### 11.3.3 Add and Norm

The input and the output of a multi-head attention layer or a position-wise feed-forward network are combined by a block that contains a residual structure and a layer normalization layer.

Layer normalization is similar batch normalization, but the mean and variances are calculated along the last dimension, e.g `X.mean(axis=-1)` instead of the first batch dimension, e.g. `X.mean(axis=0)`.

```
layer = nn.LayerNorm()
layer.initialize()
batch = nn.BatchNorm()
batch.initialize()
```

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```
X = nd.array([[1,2],[2,3]])
# compute mean and variance from X in the training mode.
with autograd.record():
    print('layer norm:',layer(X), '\nbatch norm:', batch(X))
```

```
layer norm:
[[-0.99998  0.99998]
 [-0.99998  0.99998]]
<NDArray 2x2 @cpu(0)>
batch norm:
[[ -0.99998 -0.99998]
 [ 0.99998  0.99998]]
<NDArray 2x2 @cpu(0)>
```

The connection block accepts two inputs  $X$  and  $Y$ , the input and output of an other block. Within this connection block, we apply dropout on  $Y$ .

```
class AddNorm(nn.Block):
    def __init__(self, dropout, **kwargs):
        super(AddNorm, self).__init__(**kwargs)
        self.dropout = nn.Dropout(dropout)
        self.norm = nn.LayerNorm()

    def forward(self, X, Y):
        return self.norm(self.dropout(Y) + X)
```

Due to the residual connection,  $X$  and  $Y$  should have the same shape.

```
add_norm = AddNorm(0.5)
add_norm.initialize()
add_norm(nd.ones((2,3,4)), nd.ones((2,3,4))).shape
```

```
(2, 3, 4)
```

### 11.3.4 Positional Encoding

Unlike the recurrent layer, both the multi-head attention layer and the position-wise feed-forward network compute the output of each item in the sequence independently. This property allows us to parallel the computation but is inefficient to model the sequence information. The transformer model therefore adds positional information into the input sequence.

Assume  $X \in \mathbb{R}^{l \times d}$  is the embedding of an example, where  $l$  is the sequence length and  $d$  is the embedding size. This layer will create a positional encoding  $P \in \mathbb{R}^{l \times d}$  and output  $P + X$ , with  $P$  defined as following:

$$P_{i,2j} = \sin(i/10000^{2j/d}), \quad P_{i,2j+1} = \cos(i/10000^{2j/d}), \quad (11.3.3)$$

for  $i = 0, \dots, l - 1$  and  $j = 0, \dots, \lfloor (d - 1)/2 \rfloor$ .

```
class PositionalEncoding(nn.Block):
    def __init__(self, units, dropout, max_len=1000):
        super(PositionalEncoding, self).__init__()
```

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```

self.dropout = nn.Dropout(dropout)
# Create a long enough P
self.P = nd.zeros((1, max_len, units))
X = nd.arange(0, max_len).reshape((-1,1)) / nd.power(
    10000, nd.arange(0, units, 2)/units)
self.P[:, :, 0::2] = nd.sin(X)
self.P[:, :, 1::2] = nd.cos(X)

def forward(self, X):
    X = X + self.P[:, :, :X.shape[1], :].as_in_context(X.context)
    return self.dropout(X)

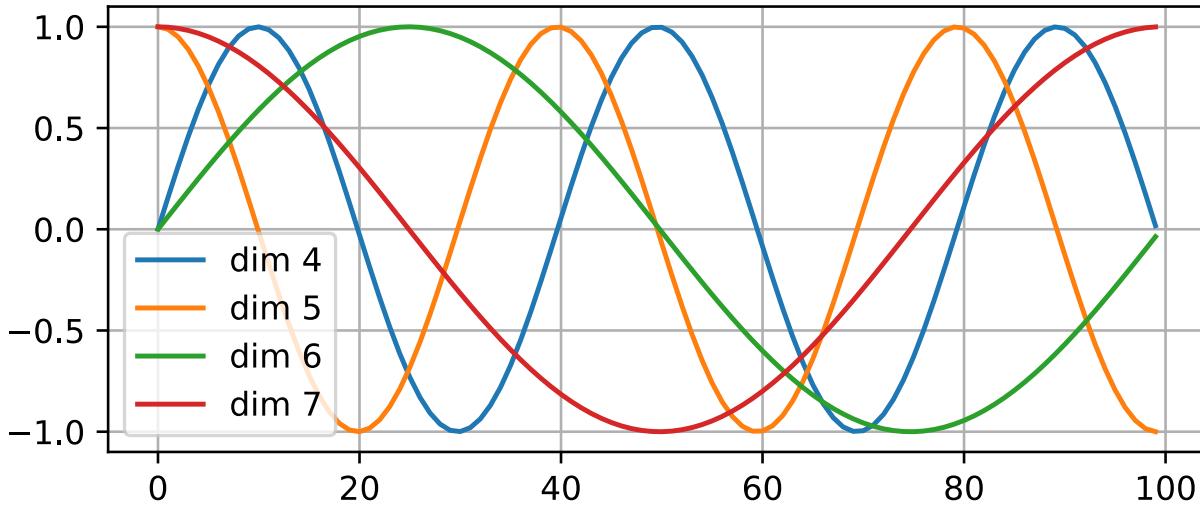
```

Now we visualize the position values for 4 dimensions. As can be seen, the 4th dimension has the same frequency as the 5th but with different offset. The 5th and 6th dimension have a lower frequency.

```

pe = PositionalEncoding(20, 0)
pe.initialize()
Y = pe(nd.zeros((1, 100, 20)))
d2l.plot(nd.arange(100), Y[0, :, 4:8].T, figsize=(6, 2.5),
         legend=["dim %d"%p for p in [4,5,6,7]])

```



### 11.3.5 Encoder

Now we define the transformer block for the encoder, which contains a multi-head attention layer, a position-wise feed-forward network, and two connection blocks.

```

class EncoderBlock(nn.Block):
    def __init__(self, units, hidden_size, num_heads, dropout, **kwargs):
        super(EncoderBlock, self).__init__(**kwargs)
        self.attention = MultiHeadAttention(units, num_heads, dropout)
        self.add_1 = AddNorm(dropout)
        self.ffn = PositionWiseFFN(units, hidden_size)
        self.add_2 = AddNorm(dropout)

```

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```
def forward(self, X, valid_length):
    Y = self.add_1(X, self.attention(X, X, X, valid_length))
    return self.add_2(Y, self.ffn(Y))
```

Due to the residual connections, this block will not change the input shape. It means the `units` argument should be equal to the input's last dimension size.

```
encoder_blk = EncoderBlock(24, 48, 8, 0.5)
encoder_blk.initialize()
encoder_blk(nd.ones((2, 100, 24)), valid_length).shape
```

```
(2, 100, 24)
```

The encoder stacks  $n$  blocks. Due to the residual connection again, the embedding layer size  $d$  is same as the transformer block output size. Also note that we multiple the embedding output by  $\sqrt{d}$  to avoid its values are too small compared to positional encodings.

```
class TransformerEncoder(d2l.Encoder):
    def __init__(self, vocab_size, units, hidden_size,
                 num_heads, num_layers, dropout, **kwargs):
        super(TransformerEncoder, self).__init__(**kwargs)
        self.units = units
        self.embed = nn.Embedding(vocab_size, units)
        self.pos_encoding = PositionalEncoding(units, dropout)
        self.blks = nn.Sequential()
        for i in range(num_layers):
            self.blks.add(
                EncoderBlock(units, hidden_size, num_heads, dropout))

    def forward(self, X, valid_length, *args):
        X = self.pos_encoding(self.embed(X) * math.sqrt(self.units))
        for blk in self.blks:
            X = blk(X, valid_length)
        return X
```

Create an encoder with two transformer blocks, whose hyper-parameters are same as before.

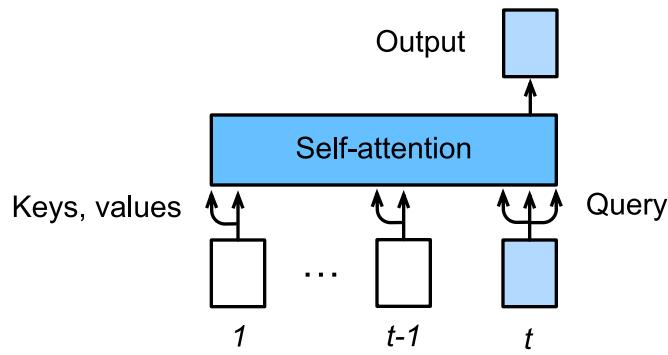
```
encoder = TransformerEncoder(200, 24, 48, 8, 2, 0.5)
encoder.initialize()
encoder(nd.ones((2, 100)), valid_length).shape
```

```
(2, 100, 24)
```

### 11.3.6 Decoder

Let first look at how a decoder behaviors during predicting. Similar to the seq2seq model, we call  $T$  forwards to generate a  $T$  length sequence. At time step  $t$ , assume  $\mathbf{x}_t$  is the current input, i.e. the query. Then keys and values of the self-attention layer consist of the current query with all past queries  $\mathbf{x}_1, \dots, \mathbf{x}_{t-1}$ .

During training, because the output for the  $t$ -query could depend all  $T$  key-value pairs, which results in an inconsistent behavior than prediction. We can eliminate it by specifying the valid length to be  $t$  for the  $t$ -th

Fig. 11.3.4: Predict at time step  $t$  for a self-attention layer.

query.

Another difference compared to the encoder transformer block is that the decoder block has an additional multi-head attention layer that accepts the encoder outputs as keys and values.

```
class DecoderBlock(nn.Block):
    # i means it's the i-th block in the decoder
    def __init__(self, units, hidden_size, num_heads, dropout, i, **kwargs):
        super(DecoderBlock, self).__init__(**kwargs)
        self.i = i
        self.attention_1 = MultiHeadAttention(units, num_heads, dropout)
        self.add_1 = AddNorm(dropout)
        self.attention_2 = MultiHeadAttention(units, num_heads, dropout)
        self.add_2 = AddNorm(dropout)
        self.ffn = PositionWiseFFN(units, hidden_size)
        self.add_3 = AddNorm(dropout)

    def forward(self, X, state):
        enc_outputs, enc_valid_lengh = state[0], state[1]
        # state[2][i] contains the past queries for this block
        if state[2][self.i] is None:
            key_values = X
        else:
            key_values = nd.concat(state[2][self.i], X, dim=1)
        state[2][self.i] = key_values
        if autograd.is_training():
            batch_size, seq_len, _ = X.shape
            # shape: (batch_size, seq_len), the values in the j-th column
            # are j+1
            valid_length = nd.arange(
                1, seq_len+1, ctx=X.context).tile((batch_size, 1))
        else:
            valid_length = None

        X2 = self.attention_1(X, key_values, key_values, valid_length)
        Y = self.add_1(X, X2)
        Y2 = self.attention_2(Y, enc_outputs, enc_outputs, enc_valid_lengh)
        Z = self.add_2(Y, Y2)
        return self.add_3(Z, self.ffn(Z)), state
```

Similar to the encoder block, `units` should be equal to the last dimension size of  $X$ .

```
decoder_blk = DecoderBlock(24, 48, 8, 0.5, 0)
decoder_blk.initialize()
X = nd.ones((2, 100, 24))
state = [encoder_blk(X, valid_length), valid_length, [None]]
decoder_blk(X, state)[0].shape
```

```
(2, 100, 24)
```

The construction of the decoder is identical to the encoder except for the additional last dense layer to obtain confident scores.

```
class TransformerDecoder(d2l.Decoder):
    def __init__(self, vocab_size, units, hidden_size,
                 num_heads, num_layers, dropout, **kwargs):
        super(TransformerDecoder, self).__init__(**kwargs)
        self.units = units
        self.num_layers = num_layers
        self.embed = nn.Embedding(vocab_size, units)
        self.pos_encoding = PositionalEncoding(units, dropout)
        self.blks = nn.Sequential()
        for i in range(num_layers):
            self.blks.add(
                DecoderBlock(units, hidden_size, num_heads, dropout, i))
        self.dense = nn.Dense(vocab_size, flatten=False)

    def init_state(self, enc_outputs, env_valid_lengh, *args):
        return [enc_outputs, env_valid_lengh, [None]*self.num_layers]

    def forward(self, X, state):
        X = self.pos_encoding(self.embed(X) * math.sqrt(self.units))
        for blk in self.blks:
            X, state = blk(X, state)
        return self.dense(X), state
```

### 11.3.7 Training

We use similar hyper-parameters as for the seq2seq with attention model: two transformer blocks with both the embedding size and the block output size to be 32. The additional hyper-parameters are chosen as 4 heads with the hidden size to be 2 times larger than output size.

```
embed_size, units, num_layers, dropout = 32, 32, 2, 0.0
batch_size, num_steps = 64, 10
lr, num_epochs, ctx = 0.005, 100, d2l.try_gpu()
num_hiddens, num_heads = 64, 4

src_vocab, tgt_vocab, train_iter = d2l.load_data_nmt(batch_size, num_steps)

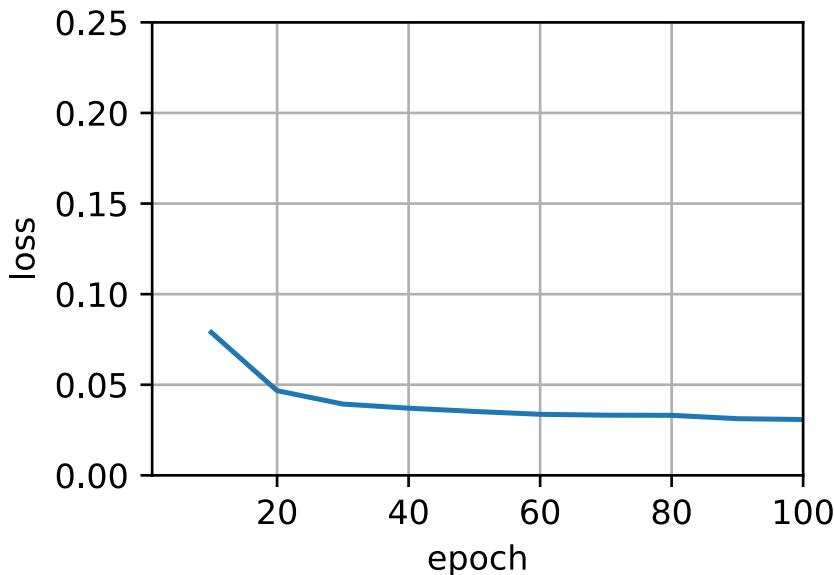
encoder = TransformerEncoder(
    len(src_vocab), units, num_hiddens, num_heads, num_layers, dropout)
decoder = TransformerDecoder(
```

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```
len(src_vocab), units, num_hiddens, num_heads, num_layers, dropout)
model = d2l.EncoderDecoder(encoder, decoder)
d2l.train_s2s_ch8(model, train_iter, lr, num_epochs, ctx)
```

```
loss 0.031, 4836 tokens/sec on gpu(0)
```



Compared to the seq2seq model with attention model, the transformer runs faster per epoch, and converges faster at the beginning.

Finally, we translate three sentences.

```
for sentence in ['Go .', 'Wow !', "I'm OK .", 'I won !']:
    print(sentence + ' => ' + d2l.predict_s2s_ch8(
        model, sentence, src_vocab, tgt_vocab, num_steps, ctx))
```

```
Go . => va !
Wow ! => <unk> !
I'm OK . => je vais bien .
I won ! => j'ai gagné !
```

### 11.3.8 Summary

- Transformer model is based on  $N \times N$  encoder-decoder architecture. It differs from Seq2seq with attention in 3 major places.
- Multi-head attention layer contains  $h$  parallel attention layers.
- Position-wise feed-forward network equals to apply 2  $Conv(1, 1)$  layers.
- Layer normalization differs from batch normalization by normalizing along the last dimension (the feature dimension) instead of the first (batchsize) dimension.
- Positional encoding is the only place that adds positional information to the transformer model.

## OPTIMIZATION ALGORITHMS

If you read the book in sequence up to this point you already used a number of advanced optimization algorithms to train deep learning models. They were the tools that allowed us to continue updating model parameters and to minimize the value of the loss function, as evaluated on the training set. Indeed, anyone content with treating optimization as a black box device to minimize objective functions in a simple setting might well content oneself with the knowledge that there exists an array of incantations of such a procedure (with names such as ‘Adam’, ‘NAG’, or ‘SGD’).

To do well, however, some deeper knowledge is required. Optimization algorithms are important for deep learning. On one hand, training a complex deep learning model can take hours, days, or even weeks. The performance of the optimization algorithm directly affects the model’s training efficiency. On the other hand, understanding the principles of different optimization algorithms and the role of their parameters will enable us to tune the hyperparameters in a targeted manner to improve the performance of deep learning models.

In this chapter, we explore common deep learning optimization algorithms in depth. Almost all optimization problems arising in deep learning are *nonconvex*. Nonetheless, the design and analysis of algorithms in the context of convex problems has proven to be very instructive. It is for that reason that this section includes a primer on convex optimization and the proof for a very simple stochastic gradient descent algorithm on a convex objective function.

### 12.1 Optimization and Deep Learning

In this section, we will discuss the relationship between optimization and deep learning as well as the challenges of using optimization in deep learning. For a deep learning problem, we will usually define a loss function first. Once we have the loss function, we can use an optimization algorithm in attempt to minimize the loss. In optimization, a loss function is often referred to as the objective function of the optimization problem. By tradition and convention most optimization algorithms are concerned with *minimization*. If we ever need to maximize an objective there’s a simple solution - just flip the sign on the objective.

#### 12.1.1 Optimization and Estimation

Although optimization provides a way to minimize the loss function for deep learning, in essence, the goals of optimization and deep learning are fundamentally different. The former is primarily concerned with minimizing an objective whereas the latter is concerned with finding a suitable model, given a finite amount of data. In Section 6.4, we discussed the difference between these two goals in detail. For instance, training error and generalization error generally differ: since the objective function of the optimization algorithm is usually a loss function based on the training data set, the goal of optimization is to reduce the training error. However, the goal of statistical inference (and thus of deep learning) is to reduce the generalization error. To accomplish the latter we need to pay attention to overfitting in addition to using the optimization algorithm to reduce the training error. We begin by importing a few libraries with a function to annotate in a figure.

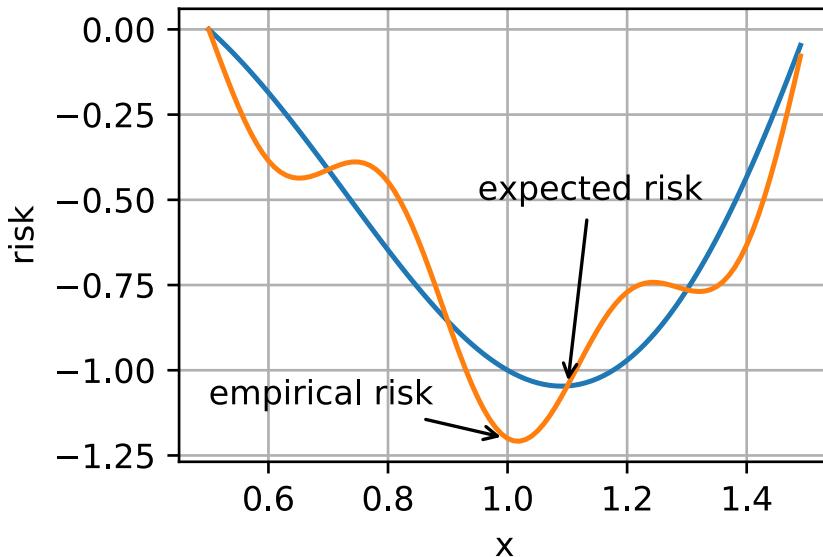
```
%matplotlib inline
import d2l
from mpl_toolkits import mplot3d
import numpy as np

# Save to the d2l package.
def annotate(text, xy, xytext):
    d2l.plt.gca().annotate(text, xy=xy, xytext=xytext,
                           arrowprops=dict(arrowstyle='->'))
```

The graph below illustrates the issue in some more detail. Since we have only a finite amount of data the minimum of the training error may be at a different location than the minimum of the expected error (or of the test error).

```
def f(x): return x * np.cos(np.pi * x)
def g(x): return f(x) + 0.2 * np.cos(5 * np.pi * x)

d2l.set_figsize((4.5, 2.5))
x = np.arange(0.5, 1.5, 0.01)
d2l.plot(x, [f(x), g(x)], 'x', 'risk')
annotate('empirical risk', (1.0, -1.2), (0.5, -1.1))
annotate('expected risk', (1.1, -1.05), (0.95, -0.5))
```



### 12.1.2 Optimization Challenges in Deep Learning

In this chapter, we are going to focus specifically on the performance of the optimization algorithm in minimizing the objective function, rather than a model's generalization error. In Section 5.1 we distinguished between analytical solutions and numerical solutions in optimization problems. In deep learning, most objective functions are complicated and do not have analytical solutions. Instead, we must use numerical optimization algorithms. The optimization algorithms below all fall into this category.

There are many challenges in deep learning optimization. Some of the most vexing ones are local minima, saddle points and vanishing gradients. Let's have a look at a few of them.

## Local Minima

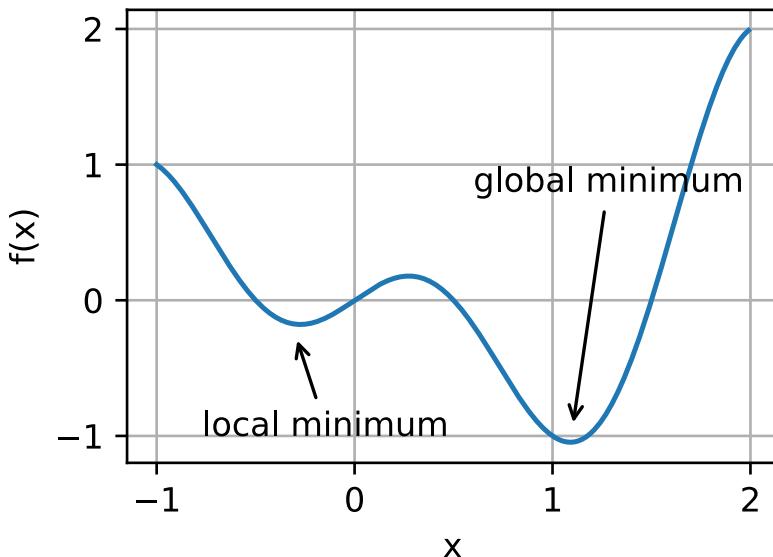
For the objective function  $f(x)$ , if the value of  $f(x)$  at  $x$  is smaller than the values of  $f(x)$  at any other points in the vicinity of  $x$ , then  $f(x)$  could be a local minimum. If the value of  $f(x)$  at  $x$  is the minimum of the objective function over the entire domain, then  $f(x)$  is the global minimum.

For example, given the function

$$f(x) = x \cdot \cos(\pi x) \text{ for } -1.0 \leq x \leq 2.0, \quad (12.1.1)$$

we can approximate the local minimum and global minimum of this function.

```
x = np.arange(-1.0, 2.0, 0.01)
d2l.plot(x, [f(x), ], 'x', 'f(x)')
annotate('local minimum', (-0.3, -0.25), (-0.77, -1.0))
annotate('global minimum', (1.1, -0.95), (0.6, 0.8))
```



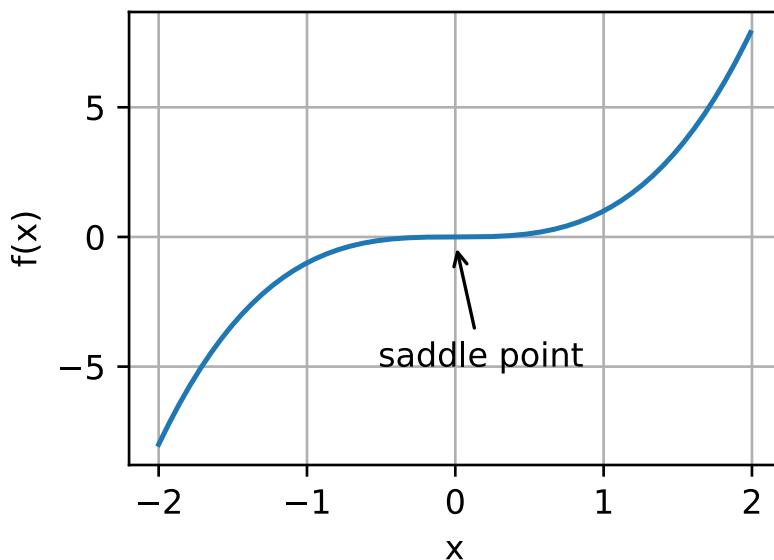
The objective function of deep learning models usually has many local optima. When the numerical solution of an optimization problem is near the local optimum, the numerical solution obtained by the final iteration may only minimize the objective function locally, rather than globally, as the gradient of the objective function's solutions approaches or becomes zero. Only some degree of noise might knock the parameter out of the local minimum. In fact, this is one of the beneficial properties of stochastic gradient descent where the natural variation of gradients over minibatches is able to dislodge the parameters from local minima.

## Saddle Points

Besides local minima, saddle points are another reason for gradients to vanish. A [saddle point](#)<sup>158</sup> is any location where all gradients of a function vanish but which is neither a global nor a local minimum. Consider the function  $f(x) = x^3$ . Its first and second derivative vanish for  $x = 0$ . Optimization might stall at the point, even though it is not a minimum.

```
x = np.arange(-2.0, 2.0, 0.01)
d2l.plot(x, [x**3], 'x', 'f(x)')
annotate('saddle point', (0, -0.2), (-0.52, -5.0))
```

<sup>158</sup> [https://en.wikipedia.org/wiki/Saddle\\_point](https://en.wikipedia.org/wiki/Saddle_point)

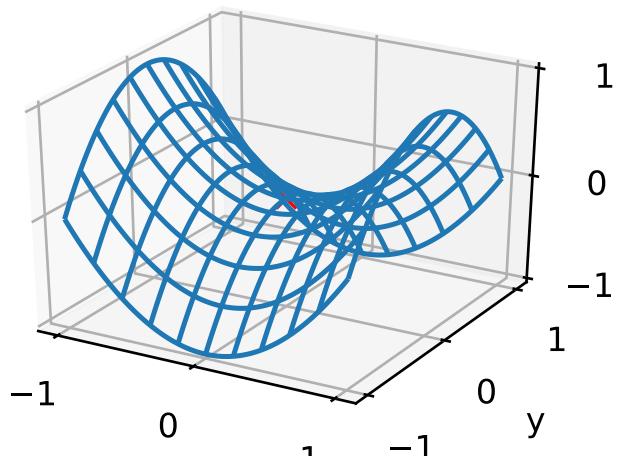


Saddle points in higher dimensions are even more insidious, as the example below shows. Consider the function  $f(x, y) = x^2 - y^2$ . It has its saddle point at  $(0, 0)$ . This is a maximum with respect to  $y$  and a minimum with respect to  $x$ . Moreover, it *looks* like a saddle, which is where this mathematical property got its name.

```
x, y = np.mgrid[-1: 1: 101j, -1: 1: 101j]

z = x**2 - y**2

ax = d2l.plt.figure().add_subplot(111, projection='3d')
ax.plot_wireframe(x, y, z, **{'rstride': 10, 'cstride': 10})
ax.plot([0], [0], [0], 'rx')
ticks = [-1, 0, 1]
d2l.plt.xticks(ticks)
d2l.plt.yticks(ticks)
ax.set_zticks(ticks)
d2l.plt.xlabel('x')
d2l.plt.ylabel('y');
```



We assume that the input of a function is a  $k$ -dimensional vector and its output is a scalar, so its Hessian matrix will have  $k$  eigenvalues (refer to [Section 17.2](#)). The solution of the function could be a local minimum, a local maximum, or a saddle point at a position where the function gradient is zero:

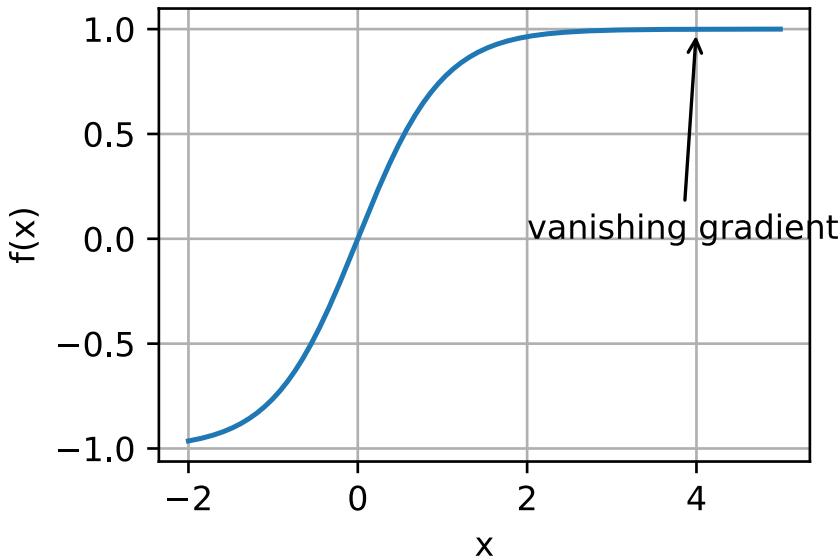
- When the eigenvalues of the function's Hessian matrix at the zero-gradient position are all positive, we have a local minimum for the function.
- When the eigenvalues of the function's Hessian matrix at the zero-gradient position are all negative, we have a local maximum for the function.
- When the eigenvalues of the function's Hessian matrix at the zero-gradient position are negative and positive, we have a saddle point for the function.

For high-dimensional problems the likelihood that at least some of the eigenvalues are negative is quite high. This makes saddle points more likely than local minima. We will discuss some exceptions to this situation in the next section when introducing convexity. In short, convex functions are those where the eigenvalues of the Hessian are never negative. Sadly, though, most deep learning problems do not fall into this category. Nonetheless it's a great tool to study optimization algorithms.

### Vanishing Gradients

Probably the most insidious problem to encounter are vanishing gradients. For instance, assume that we want to minimize the function  $f(x) = \tanh(x)$  and we happen to get started at  $x = 4$ . As we can see, the gradient of  $f$  is close to nil. More specifically  $f'(x) = 1 - \tanh^2(x)$  and thus  $f'(4) = 0.0013$ . Consequently optimization will get stuck for a long time before we make progress. This turns out to be one of the reasons that training deep learning models was quite tricky prior to the introduction of the ReLU activation function.

```
x = np.arange(-2.0, 5.0, 0.01)
d2l.plot(x, [np.tanh(x)], 'x', 'f(x)')
annotate('vanishing gradient', (4, 1), (2, 0.0))
```



As we saw, optimization for deep learning is full of challenges. Fortunately there exists a robust range of algorithms that perform well and that are easy to use even for beginners. Furthermore, it isn't really necessary to find *the* best solution. Local optima or even approximate solutions thereof are still very useful.

### 12.1.3 Summary

- Minimizing the training error does *not* guarantee that we find the best set of parameters to minimize the expected error.
- The optimization problems may have many local minima.
- The problem may have even more saddle points, as generally the problems are not convex.
- Vanishing gradients can cause optimization to stall. Often a reparametrization of the problem helps. Good initialization of the parameters can be beneficial, too.

### 12.1.4 Exercises

1. Consider a simple multilayer perceptron with a single hidden layer of, say,  $d$  dimensions in the hidden layer and a single output. Show that for any local minimum there are at least  $d!$  equivalent solutions that behave identically.
2. Assume that we have a symmetric random matrix  $\mathbf{M}$  where the entries  $M_{ij} = M_{ji}$  are each drawn from some probability distribution  $p_{ij}$ . Furthermore assume that  $p_{ij}(x) = p_{ij}(-x)$ , i.e. that the distribution is symmetric (see e.g. [65] for details).
  - Prove that the distribution over eigenvalues is also symmetric. That is, for any eigenvector  $\mathbf{v}$  the probability that the associated eigenvalue  $\lambda$  satisfies  $\Pr(\lambda > 0) = \Pr(\lambda < 0)$ .
  - Why does the above *not* imply  $\Pr(\lambda > 0) = 0.5$ ?
3. What other challenges involved in deep learning optimization can you think of?
4. Assume that you want to balance a (real) ball on a (real) saddle.
  - Why is this hard?
  - Can you exploit this effect also for optimization algorithms?

### 12.1.5 Scan the QR Code to Discuss<sup>159</sup>



## 12.2 Convexity

Convexity plays a vital role in the design of optimization algorithms. This is largely due to the fact that it is much easier to analyze and test algorithms in this context. In other words, if the algorithm performs poorly even in the convex setting we should not hope to see great results otherwise. Furthermore, even though the optimization problems in deep learning are generally nonconvex, they often exhibit some properties of convex ones near local minima. This can lead to exciting new optimization variants such as [Stochastic Weight Averaging](#)<sup>160</sup> by Izmailov et al., 2018. Let's begin with the basics.

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<sup>159</sup> <https://discuss.mxnet.io/t/2371>

<sup>160</sup> <https://arxiv.org/abs/1803.05407>

### 12.2.1 Basics

#### Sets

Sets are the basis of convexity. Simply put, a set  $X$  in a vector space is convex if for any  $a, b \in X$  the line segment connecting  $a$  and  $b$  is also in  $X$ . In mathematical terms this means that for all  $\lambda \in [0, 1]$  we have

$$\lambda \cdot a + (1 - \lambda) \cdot b \in X \text{ whenever } a, b \in X. \quad (12.2.1)$$

This sounds a bit abstract. Consider the picture below. The first set isn't convex since there are line segments that are not contained in it. The other two sets suffer no such problem.

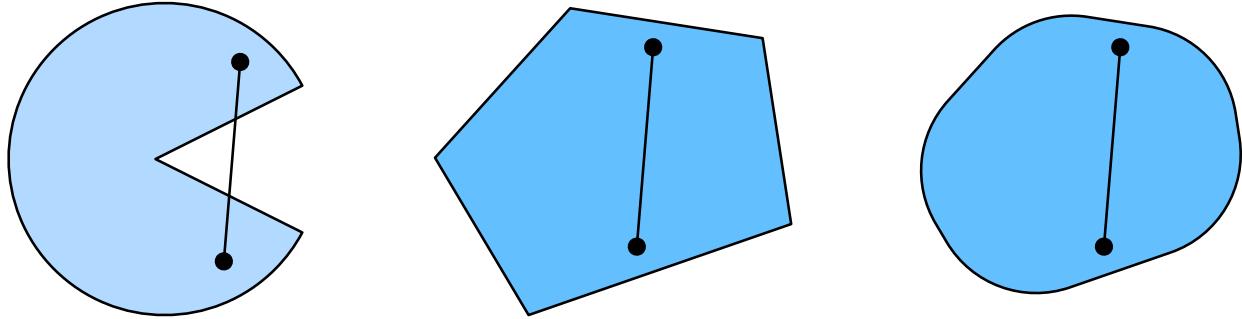


Fig. 12.2.1: Three shapes, the left one is nonconvex, the others are convex

Definitions on their own aren't particularly useful unless you can do something with them. In this case we can look at unions and intersections. Assume that  $X$  and  $Y$  are convex sets. Then  $X \cap Y$  is also convex. To see this, consider any  $a, b \in X \cap Y$ . Since  $X$  and  $Y$  are convex, the line segments connecting  $a$  and  $b$  are contained in both  $X$  and  $Y$ . Given that, they also need to be contained in  $X \cap Y$ , thus proving our first theorem.

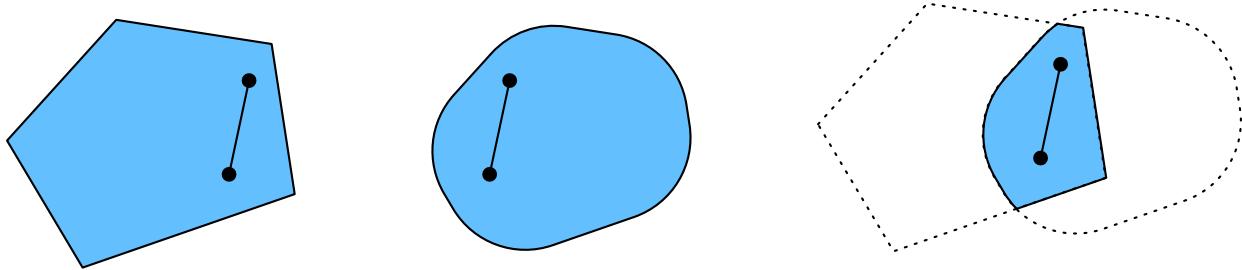


Fig. 12.2.2: The intersection between two convex sets is convex

We can strengthen this result with little effort: given convex sets  $X_i$ , their intersection  $\cap_i X_i$  is convex. To see that the converse is not true, consider two disjoint sets  $X \cap Y = \emptyset$ . Now pick  $a \in X$  and  $b \in Y$ . The line segment connecting  $a$  and  $b$  needs to contain some part that is neither in  $X$  nor  $Y$ , since we assumed that  $X \cap Y = \emptyset$ . Hence the line segment isn't in  $X \cup Y$  either, thus proving that in general unions of convex sets need not be convex.

Typically the problems in deep learning are defined on convex domains. For instance  $\mathbb{R}^d$  is a convex set (after all, the line between any two points in  $\mathbb{R}^d$  remains in  $\mathbb{R}^d$ ). In some cases we work with variables of bounded length, such as balls of radius  $r$  as defined by  $\{\mathbf{x} | \mathbf{x} \in \mathbb{R}^d \text{ and } \|\mathbf{x}\|_2 \leq r\}$ .

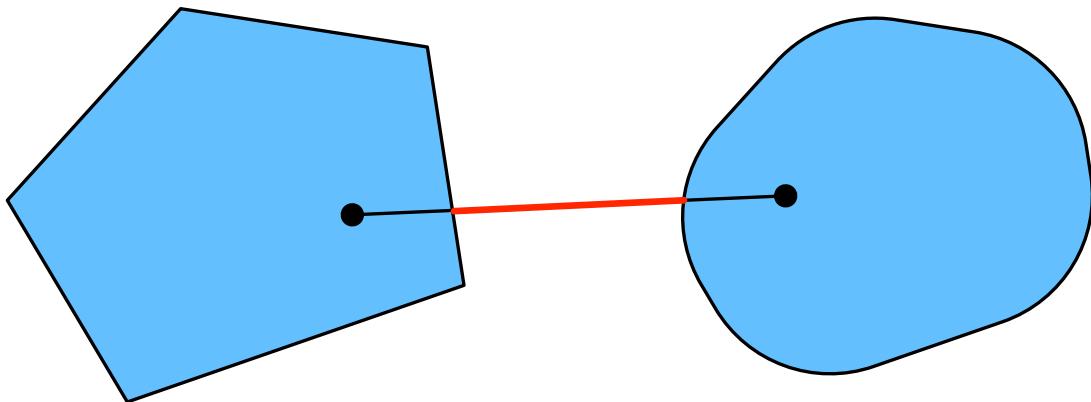


Fig. 12.2.3: The union of two convex sets need not be convex

## Functions

Now that we have convex sets we can introduce convex functions  $f$ . Given a convex set  $X$  a function defined on it  $f : X \rightarrow \mathbb{R}$  is convex if for all  $x, x' \in X$  and for all  $\lambda \in [0, 1]$  we have

$$\lambda f(x) + (1 - \lambda)f(x') \geq f(\lambda x + (1 - \lambda)x'). \quad (12.2.2)$$

To illustrate this let's plot a few functions and check which ones satisfy the requirement. We need to import a few libraries.

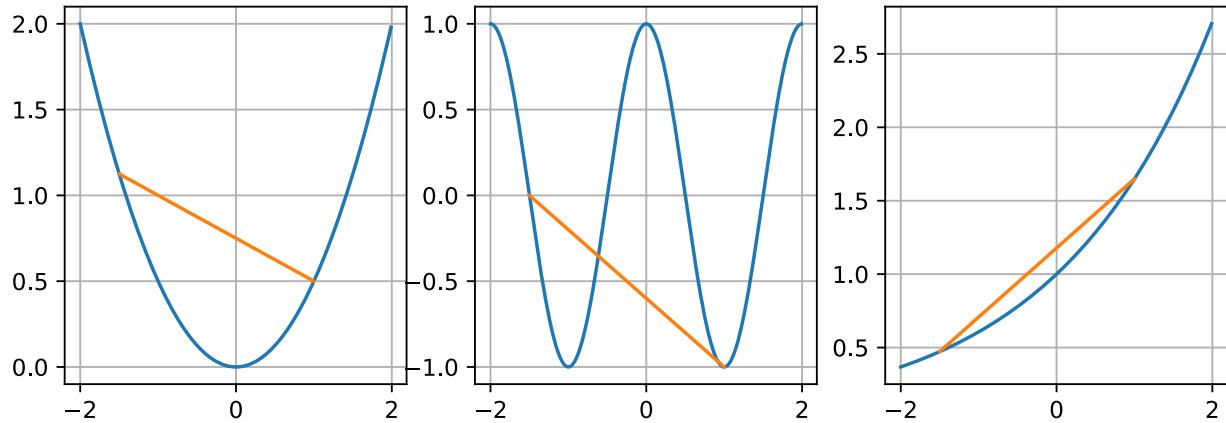
```
%matplotlib inline
import d2l
from mpl_toolkits import mplot3d
import numpy as np
```

Let's define a few functions, both convex and nonconvex.

```
def f(x): return 0.5 * x**2      # convex
def g(x): return np.cos(np.pi * x) # nonconvex
def h(x): return np.exp(0.5 * x)  # convex

x, segment = np.arange(-2, 2, 0.01), np.array([-1.5, 1])
d2l.use_svg_display()
_, axes = d2l.plt.subplots(1, 3, figsize=(9, 3))

for ax, func in zip(axes, [f, g, h]):
    d2l.plot([x, segment], [func(x), func(segment)], axes=ax)
```



As expected, the cosine function is nonconvex, whereas the parabola and the exponential function are. Note that the requirement that  $X$  is necessary for the condition to make sense. Otherwise the outcome of  $f(\lambda x + (1 - \lambda)x')$  might not be well defined. Convex functions have a number of desirable properties.

### Jensen's Inequality

One of the most useful tools is Jensen's inequality. It amounts to a generalization of the definition of convexity.

$$\sum_i \alpha_i f(x_i) \geq f\left(\sum_i \alpha_i x_i\right) \quad (12.2.3)$$

and  $\mathbf{E}_x[f(x)] \geq f(\mathbf{E}_x[x])$

In other words, the expectation of a convex function is larger than the convex function of an expectation. To prove the first inequality we repeatedly apply the definition of convexity to one term in the sum at a time. The expectation can be proven by taking the limit over finite segments.

One of the common applications of Jensen's inequality is with regard to the log-likelihood of partially observed random variables. That is, we use

$$\mathbf{E}_{y \sim p(y)}[-\log p(x|y)] \geq -\log p(x). \quad (12.2.4)$$

This follows since  $\int p(y)p(x|y)dy = p(x)$ . This is used in variational methods. Here  $y$  is typically the unobserved random variable,  $p(y)$  is the best guess of how it might be distributed and  $p(x)$  is the distribution with  $y$  integrated out. For instance, in clustering  $y$  might be the cluster labels and  $p(x|y)$  is the generative model when applying cluster labels.

## 12.2.2 Properties

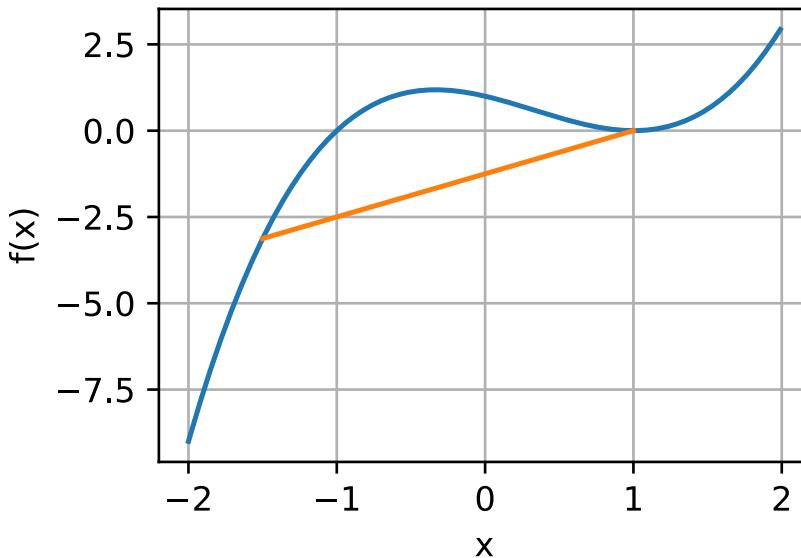
### No Local Minima

In particular, convex functions do not have local minima. Let's assume the contrary and prove it wrong. If  $x \in X$  is a local minimum there exists some neighborhood of  $x$  for which  $f(x)$  is the smallest value. Since  $x$  is only a local minimum there has to be another  $x' \in X$  for which  $f(x') < f(x)$ . However, by convexity the function values on the entire line  $\lambda x + (1 - \lambda)x'$  have to be less than  $f(x')$  since for  $\lambda \in [0, 1]$

$$f(x) > \lambda f(x) + (1 - \lambda)f(x') \geq f(\lambda x + (1 - \lambda)x'). \quad (12.2.5)$$

This contradicts the assumption that  $f(x)$  is a local minimum. For instance, the function  $f(x) = (x+1)(x-1)^2$  has a local minimum for  $x = 1$ . However, it is not a global minimum.

```
def f(x): return (x-1)**2 * (x+1)
d2l.set_figsize((3.5, 2.5))
d2l.plot([x, segment], [f(x), f(segment)], 'x', 'f(x)')
```



The fact that convex functions have no local minima is very convenient. It means that if we minimize functions we cannot ‘get stuck’. Note, though, that this doesn’t mean that there cannot be more than one global minimum or that there might even exist one. For instance, the function  $f(x) = \max(|x| - 1, 0)$  attains its minimum value over the interval  $[-1, 1]$ . Conversely, the function  $f(x) = \exp(x)$  does not attain a minimum value on  $\mathbb{R}$ . For  $x \rightarrow -\infty$  it asymptotes to 0, however there is no  $x$  for which  $f(x) = 0$ .

## Convex Functions and Sets

Convex functions define convex sets as *below-sets*. They are defined as

$$S_b := \{x | x \in X \text{ and } f(x) \leq b\}. \quad (12.2.6)$$

Such sets are convex. Let’s prove this quickly. Remember that for any  $x, x' \in S_b$  we need to show that  $\lambda x + (1 - \lambda)x' \in S_b$  as long as  $\lambda \in [0, 1]$ . But this follows directly from the definition of convexity since  $f(\lambda x + (1 - \lambda)x') \leq \lambda f(x) + (1 - \lambda)f(x') \leq b$ .

Have a look at the function  $f(x, y) = 0.5x^2 + \cos(2\pi y)$  below. It is clearly nonconvex. The level sets are correspondingly nonconvex. In fact, they’re typically composed of disjoint sets.

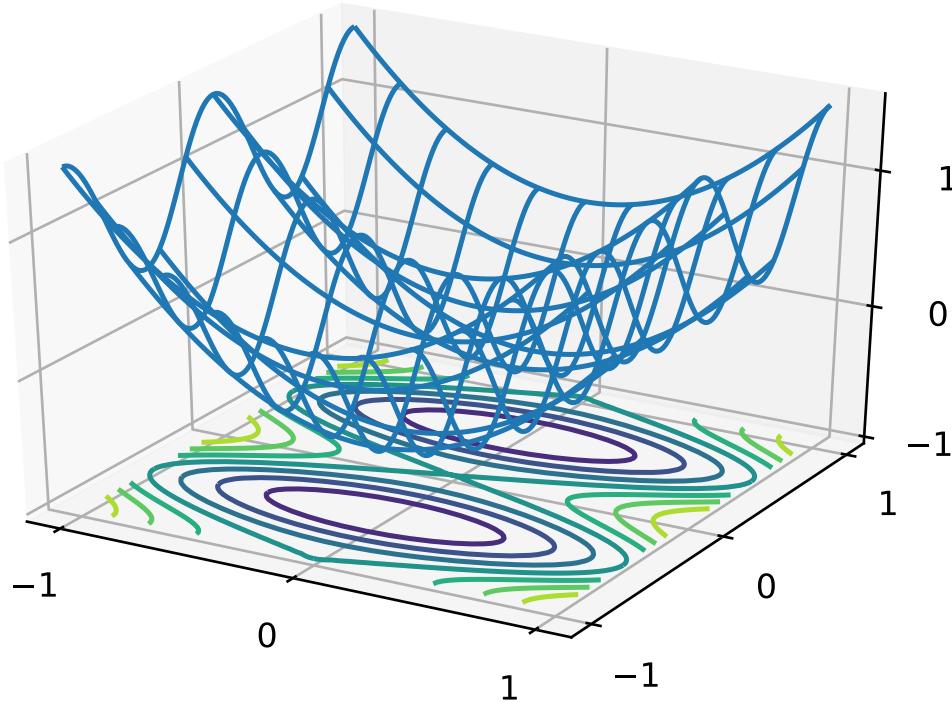
```
x, y = np.mgrid[-1: 1: 101j, -1: 1: 101j]
z = x**2 + 0.5 * np.cos(2 * np.pi * y)

# Plot the 3D surface
d2l.set_figsize((6,4))
ax = d2l.plt.figure().add_subplot(111, projection='3d')
ax.plot_wireframe(x, y, z, **{'rstride': 10, 'cstride': 10})
ax.contour(x, y, z, offset=-1)
ax.set_zlim(-1, 1.5)
```

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```
# Adjust labels
for func in [d2l.plt.xticks, d2l.plt.yticks, ax.set_zticks]: func([-1,0,1])
```



## Derivatives and Convexity

Whenever the second derivative of a function exists it is very easy to check for convexity. All we need to do is check whether  $\partial_x^2 f(x) \succeq 0$ , i.e. whether all of its eigenvalues are nonnegative. For instance, the function  $f(\mathbf{x}) = \frac{1}{2} \|\mathbf{x}\|_2^2$  is convex since  $\partial_{\mathbf{x}}^2 f = \mathbf{I}$ , i.e. its derivative is the identity matrix.

The first thing to realize is that we only need to prove this property for one-dimensional functions. After all, in general we can always define some function  $g(z) = f(\mathbf{x} + z \cdot \mathbf{v})$ . This function has the first and second derivatives  $g' = (\partial_{\mathbf{x}} f)^{\top} \mathbf{v}$  and  $g'' = \mathbf{v}^{\top} (\partial_{\mathbf{x}}^2 f) \mathbf{v}$  respectively. In particular,  $g'' \geq 0$  for all  $\mathbf{v}$  whenever the Hessian of  $f$  is positive semidefinite, i.e. whenever all of its eigenvalues are greater than or equal to zero. Hence back to the scalar case.

To see that  $f''(x) \geq 0$  for convex functions we use the fact that

$$\frac{1}{2}f(x+\epsilon) + \frac{1}{2}f(x-\epsilon) \geq f\left(\frac{x+\epsilon}{2} + \frac{x-\epsilon}{2}\right) = f(x) \quad (12.2.7)$$

Since the second derivative is given by the limit over finite differences it follows that

$$f''(x) = \lim_{\epsilon \rightarrow 0} \frac{f(x+\epsilon) + f(x-\epsilon) - 2f(x)}{\epsilon^2} \geq 0. \quad (12.2.8)$$

To see that the converse is true we use the fact that  $f'' \geq 0$  implies that  $f'$  is a monotonically increasing function. Let  $a < x < b$  be three points in  $\mathbb{R}$ . We use the mean value theorem to express

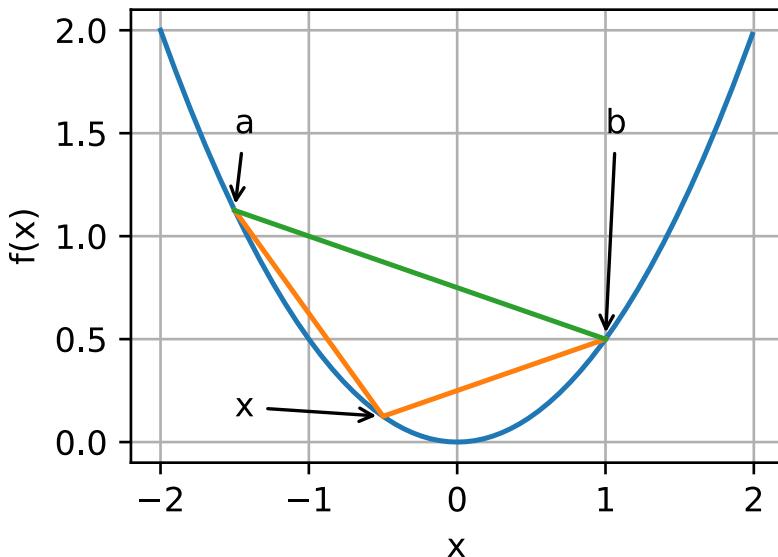
$$\begin{aligned} f(x) - f(a) &= (x-a)f'(\alpha) \text{ for some } \alpha \in [a, x] \text{ and} \\ f(b) - f(x) &= (b-x)f'(\beta) \text{ for some } \beta \in [x, b]. \end{aligned} \quad (12.2.9)$$

By monotonicity  $f'(\beta) \geq f'(\alpha)$ , hence

$$\begin{aligned} f(b) - f(a) &= f(b) - f(x) + f(x) - f(a) \\ &= (b - x)f'(\beta) + (x - a)f'(\alpha) \\ &\geq (b - a)f'(\alpha). \end{aligned} \tag{12.2.10}$$

By geometry it follows that  $f(x)$  is below the line connecting  $f(a)$  and  $f(b)$ , thus proving convexity. We omit a more formal derivation in favor of a graph below.

```
def f(x): return 0.5 * x**2
x, axb, ab = np.arange(-2, 2, 0.01), np.array([-1.5, -0.5, 1]), np.array([-1.5, 1])
d2l.set_figsize((3.5, 2.5))
d2l.plot([x, axb, ab], [f(x) for x in [x, axb, ab]], 'x', 'f(x)')
d2l.annotate('a', (-1.5, f(-1.5)), (-1.5, 1.5))
d2l.annotate('b', (1, f(1)), (1, 1.5))
d2l.annotate('x', (-0.5, f(-0.5)), (-1.5, f(-0.5)))
```



### 12.2.3 Constraints

One of the nice properties of convex optimization is that it allows us to handle constraints efficiently. That is, it allows us to solve problems of the form:

$$\begin{aligned} &\underset{\mathbf{x}}{\text{minimize}} \quad f(\mathbf{x}) \\ &\text{subject to } c_i(\mathbf{x}) \leq 0 \text{ for all } i \in \{1, \dots, N\} \end{aligned} \tag{12.2.11}$$

Here  $f$  is the objective and the functions  $c_i$  are constraint functions. To see what this does consider the case where  $c_1(\mathbf{x}) = \|\mathbf{x}\|_2 - 1$ . In this case the parameters  $\mathbf{x}$  are constrained to the unit ball. If a second constraint is  $c_2(\mathbf{x}) = \mathbf{v}^\top \mathbf{x} + b$ , then this corresponds to all  $\mathbf{x}$  lying on a halfspace. Satisfying both constraints simultaneously amounts to selecting a slice of a ball as the constraint set.

## Lagrange Function

In general, solving a constrained optimization problem is difficult. One way of addressing it stems from physics with a rather simple intuition. Imagine a ball inside a box. The ball will roll to the place that is lowest and the forces of gravity will be balanced out with the forces that the sides of the box can impose on the ball. In short, the gradient of the objective function (i.e. gravity) will be offset by the gradient of the constraint function (need to remain inside the box by virtue of the walls ‘pushing back’). Note that any constraint that is not active (i.e. the ball doesn’t touch the wall) will not be able to exert any force on the ball.

Skipping over the derivation of the Lagrange function  $L$  (see e.g. the book by Boyd and Vandenberghe, 2004<sup>161</sup> for details) the above reasoning can be expressed via the following saddlepoint optimization problem:

$$L(\mathbf{x}, \alpha) = f(\mathbf{x}) + \sum_i \alpha_i c_i(\mathbf{x}) \text{ where } \alpha_i \geq 0 \quad (12.2.12)$$

Here the variables  $\alpha_i$  are the so-called *Lagrange Multipliers* that ensure that a constraint is properly enforced. They are chosen just large enough to ensure that  $c_i(\mathbf{x}) \leq 0$  for all  $i$ . For instance, for any  $\mathbf{x}$  for which  $c_i(\mathbf{x}) < 0$  naturally, we’d end up picking  $\alpha_i = 0$ . Moreover, this is a *saddlepoint* optimization problem where one wants to *maximize*  $L$  with respect to  $\alpha$  and simultaneously *minimize* it with respect to  $\mathbf{x}$ . There is a rich body of literature explaining how to arrive at the function  $L(\mathbf{x}, \alpha)$ . For our purposes it is sufficient to know that the saddlepoint of  $L$  is where the original constrained optimization problem is solved optimally.

## Penalties

One way of satisfying constrained optimization problems at least approximately is to adapt the Lagrange function  $L$ . Rather than satisfying  $c_i(\mathbf{x}) \leq 0$  we simply add  $\alpha_i c_i(\mathbf{x})$  to the objective function  $f(x)$ . This ensures that the constraints won’t be violated too badly.

In fact, we’ve been using this trick all along. Consider weight decay in Section 6.5. In it we add  $\frac{\lambda}{2} \|\mathbf{w}\|^2$  to the objective function to ensure that  $\mathbf{w}$  doesn’t grow too large. Using the constrained optimization point of view we can see that this will ensure that  $\|\mathbf{w}\|^2 - r^2 \leq 0$  for some radius  $r$ . Adjusting the value of  $\lambda$  allows us to vary the size of  $\mathbf{w}$ .

In general, adding penalties is a good way of ensuring approximate constraint satisfaction. In practice this turns out to be much more robust than exact satisfaction. Furthermore, for nonconvex problems many of the properties that make the exact approach so appealing in the convex case (e.g. optimality) no longer hold.

## Projections

An alternative strategy for satisfying constraints are projections. Again, we encountered them before, e.g. when dealing with gradient clipping in Section 10.5. There we ensured that a gradient has length bounded by  $c$  via

$$\mathbf{g} \leftarrow \mathbf{g} \cdot \min(1, c/\|\mathbf{g}\|). \quad (12.2.13)$$

This turns out to be a *projection* of  $g$  onto the ball of radius  $c$ . More generally, a projection on a (convex) set  $X$  is defined as

$$\text{Proj}_X(\mathbf{x}) = \operatorname{argmin}_{\mathbf{x}' \in X} \|\mathbf{x} - \mathbf{x}'\|_2 \quad (12.2.14)$$

It is thus the closest point in  $X$  to  $\mathbf{x}$ . This sounds a bit abstract. The figure below explains it somewhat more clearly. In it we have two convex sets, a circle and a diamond. Points inside the set (yellow) remain unchanged. Points outside the set (black) are mapped to the closest point inside the set (red). While for  $\ell_2$

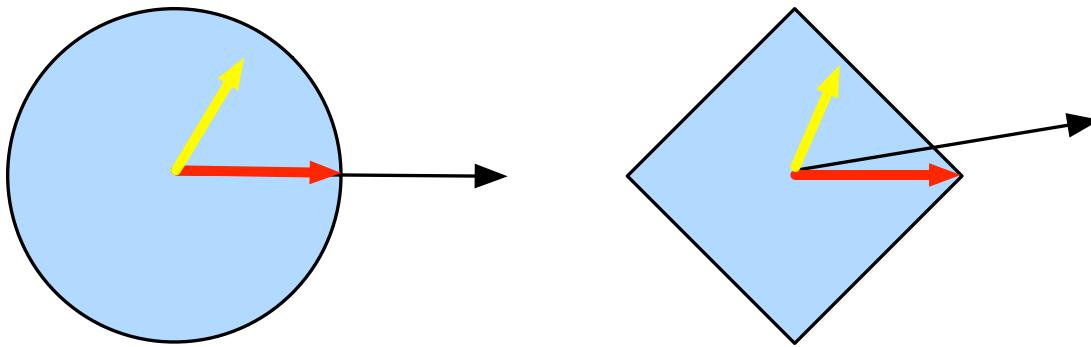


Fig. 12.2.4: Convex Projections

balls this leaves the direction unchanged, this need not be the case in general, as can be seen in the case of the diamond.

One of the uses for convex projections is to compute sparse weight vectors. In this case we project  $\mathbf{w}$  onto an  $\ell_1$  ball (the latter is a generalized version of the diamond in the picture above).

#### 12.2.4 Summary

In the context of deep learning the main purpose of convex functions is to motivate optimization algorithms and help us understand them in detail. In the following we will see how gradient descent and stochastic gradient descent can be derived accordingly.

- Intersections of convex sets are convex. Unions are not.
- The expectation of a convex function is larger than the convex function of an expectation (Jensen's inequality).
- A twice-differentiable function is convex if and only if its second derivative has only nonnegative eigenvalues throughout.
- Convex constraints can be added via the Lagrange function. In practice simply add them with a penalty to the objective function.
- Projections map to points in the (convex) set closest to the original point.

#### 12.2.5 Exercises

1. Assume that we want to verify convexity of a set by drawing all lines between points within the set and checking whether the lines are contained.
  - Prove that it is sufficient to check only the points on the boundary.
  - Prove that it is sufficient to check only the vertices of the set.
2. Denote by  $B_p[r] := \{\mathbf{x} | \mathbf{x} \in \mathbb{R}^d \text{ and } \|\mathbf{x}\|_p \leq r\}$  the ball of radius  $r$  using the  $p$ -norm. Prove that  $B_p[r]$  is convex for all  $p \geq 1$ .
3. Given convex functions  $f$  and  $g$  show that  $\max(f, g)$  is convex, too. Prove that  $\min(f, g)$  is not convex.
4. Prove that the normalization of the softmax function is convex. More specifically prove the convexity of  $f(x) = \log \sum_i \exp(x_i)$ .

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<sup>161</sup> [https://web.stanford.edu/~boyd/cvxbook/bv\\_cvxbook.pdf](https://web.stanford.edu/~boyd/cvxbook/bv_cvxbook.pdf)

5. Prove that linear subspaces are convex sets, i.e.  $X = \{\mathbf{x} | \mathbf{W}\mathbf{x} = \mathbf{b}\}$ .
6. Prove that in the case of linear subspaces with  $\mathbf{b} = 0$  the projection  $\text{Proj}_X$  can be written as  $\mathbf{M}\mathbf{x}$  for some matrix  $\mathbf{M}$ .
7. Show that for convex twice differentiable functions  $f$  we can write  $f(x+\epsilon) = f(x) + \epsilon f'(x) + \frac{1}{2}\epsilon^2 f''(x+\xi)$  for some  $\xi \in [0, \epsilon]$ .
8. Given a vector  $\mathbf{w} \in \mathbb{R}^d$  with  $\|\mathbf{w}\|_1 > 1$  compute the projection on the  $\ell_1$  unit ball.
  - As intermediate step write out the penalized objective  $\|\mathbf{w} - \mathbf{w}'\|_2^2 + \lambda \|\mathbf{w}'\|_1$  and compute the solution for a given  $\lambda > 0$ .
  - Can you find the ‘right’ value of  $\lambda$  without a lot of trial and error?
9. Given a convex set  $X$  and two vectors  $\mathbf{x}$  and  $\mathbf{y}$  prove that projections never increase distances, i.e.  $\|\mathbf{x} - \mathbf{y}\| \geq \|\text{Proj}_X(\mathbf{x}) - \text{Proj}_X(\mathbf{y})\|$ .

## 12.3 Gradient Descent

In this section we are going to introduce the basic concepts underlying gradient descent. This is brief by necessity. See e.g. [6] for an in-depth introduction to convex optimization. Although the latter is rarely used directly in deep learning, an understanding of gradient descent is key to understanding stochastic gradient descent algorithms. For instance, the optimization problem might diverge due to an overly large learning rate. This phenomenon can already be seen in gradient descent. Likewise, preconditioning is a common technique in gradient descent and carries over to more advanced algorithms. Let’s start with a simple special case.

### 12.3.1 Gradient Descent in One Dimension

Gradient descent in one dimension is an excellent example to explain why the gradient descent algorithm may reduce the value of the objective function. Consider some continuously differentiable real-valued function  $f : \mathbb{R} \rightarrow \mathbb{R}$ . Using a Taylor expansion (Section 17.2) we obtain that

$$f(x + \epsilon) = f(x) + \epsilon f'(x) + O(\epsilon^2). \quad (12.3.1)$$

That is, in first approximation  $f(x + \epsilon)$  is given by the function value  $f(x)$  and the first derivative  $f'(x)$  at  $x$ . It is not unreasonable to assume that for small  $\epsilon$  moving in the direction of the negative gradient will decrease  $f$ . To keep things simple we pick a fixed step size  $\eta > 0$  and choose  $\epsilon = -\eta f'(x)$ . Plugging this into the Taylor expansion above we get

$$f(x - \eta f'(x)) = f(x) - \eta f'^2(x) + O(\eta^2 f'^2(x)). \quad (12.3.2)$$

If the derivative  $f'(x) \neq 0$  does not vanish we make progress since  $\eta f'^2(x) > 0$ . Moreover, we can always choose  $\eta$  small enough for the higher order terms to become irrelevant. Hence we arrive at

$$f(x - \eta f'(x)) \lesssim f(x). \quad (12.3.3)$$

This means that, if we use

$$x \leftarrow x - \eta f'(x) \quad (12.3.4)$$

to iterate  $x$ , the value of function  $f(x)$  might decline. Therefore, in gradient descent we first choose an initial value  $x$  and a constant  $\eta > 0$  and then use them to continuously iterate  $x$  until the stop condition is reached, for example, when the magnitude of the gradient  $|f'(x)|$  is small enough or the number of iterations has reached a certain value.

For simplicity we choose the objective function  $f(x) = x^2$  to illustrate how to implement gradient descent. Although we know that  $x = 0$  is the solution to minimize  $f(x)$ , we still use this simple function to observe how  $x$  changes. As always, we begin by importing all required modules.

```
%matplotlib inline
import d2l
import numpy as np
import math

def f(x):      return x**2 # objective function
def gradf(x): return 2 * x # its derivative
```

Next, we use  $x = 10$  as the initial value and assume  $\eta = 0.2$ . Using gradient descent to iterate  $x$  for 10 times we can see that, eventually, the value of  $x$  approaches the optimal solution.

```
def gd(eta):
    x = 10
    results = [x]
    for i in range(10):
        x -= eta * gradf(x)
        results.append(x)
    print('epoch 10, x:', x)
    return results

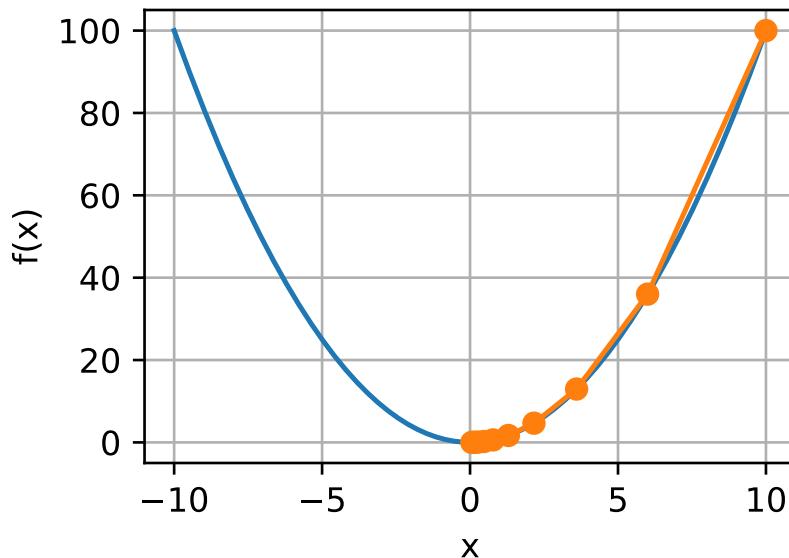
res = gd(0.2)
```

```
epoch 10, x: 0.06046617599999997
```

The progress of optimizing over  $x$  can be plotted as follows.

```
def show_trace(res):
    n = max(abs(min(res)), abs(max(res)))
    f_line = np.arange(-n, n, 0.01)
    d2l.set_figsize((3.5, 2.5))
    d2l.plot([f_line, res], [[f(x) for x in f_line], [f(x) for x in res]],
             'x', 'f(x)', fmts=['-', '-o'])

show_trace(res)
```

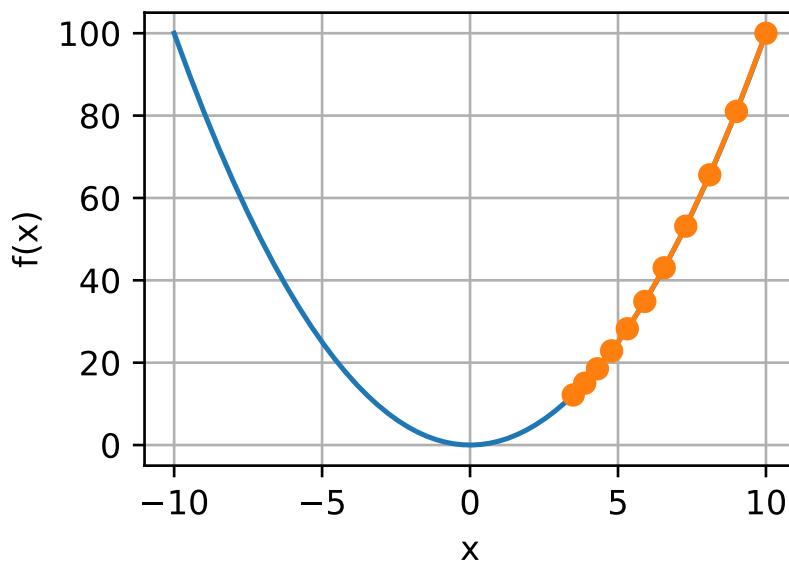


### Learning Rate

The learning rate  $\eta$  can be set by the algorithm designer. If we use a learning rate that is too small, it will cause  $x$  to update very slowly, requiring more iterations to get a better solution. To show what happens in such a case, consider the progress in the same optimization problem for  $\eta = 0.05$ . As we can see, even after 10 steps we are still very far from the optimal solution.

```
show_trace(gd(0.05))
```

```
epoch 10, x: 3.4867844009999995
```

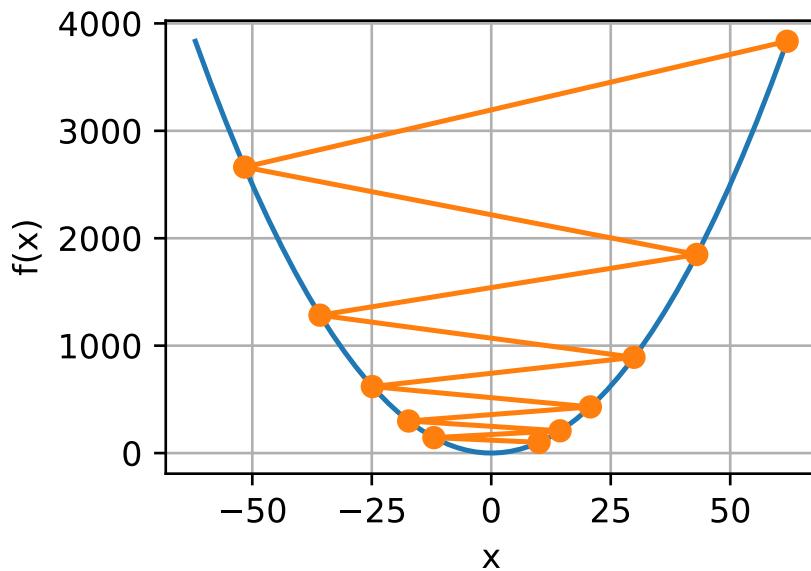


Conversely, if we use an excessively high learning rate,  $|\eta f'(x)|$  might be too large for the first-order Taylor expansion formula. That is, the term  $O(\eta^2 f'^2(x))$  in (12.3.1) might become significant. In this case, we

cannot guarantee that the iteration of  $x$  will be able to lower the value of  $f(x)$ . For example, when we set the learning rate to  $\eta = 1.1$ ,  $x$  overshoots the optimal solution  $x = 0$  and gradually diverges.

```
show_trace(gd(1.1))
```

```
epoch 10, x: 61.917364224000096
```



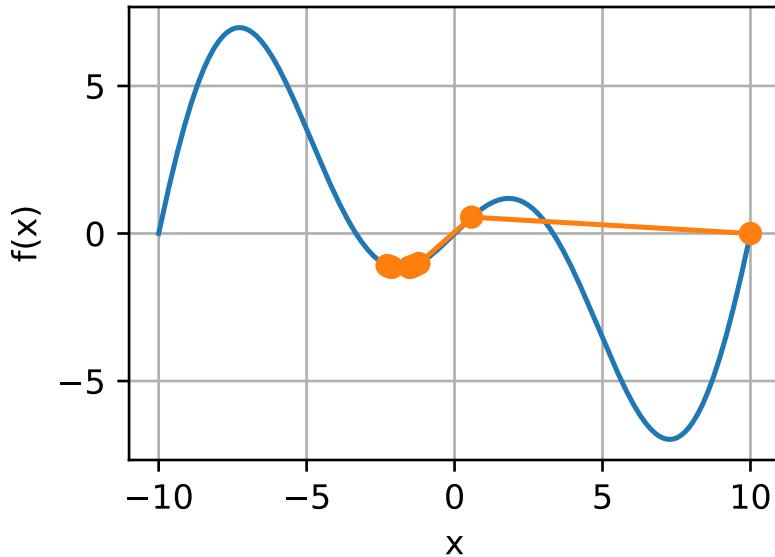
### Local Minima

To illustrate what happens for nonconvex functions consider the case of  $f(x) = x \cdot \cos cx$ . This function has infinitely many local minima. Depending on our choice of learning rate and depending on how well conditioned the problem is, we may end up with one of many solutions. The example below illustrates how an (unrealistically) high learning rate will lead to a poor local minimum.

```
c = 0.15 * math.pi
def f(x):      return x*math.cos(c * x)
def gradf(x):  return math.cos(c * x) - c * x * math.sin(c * x)

show_trace(gd(2))
```

```
epoch 10, x: -1.528165927635083
```



### 12.3.2 Multivariate Gradient Descent

Now that we have a better intuition of the univariate case, let us consider the situation where  $\mathbf{x} \in \mathbb{R}^d$ . That is, the objective function  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  maps vectors into scalars. Correspondingly its gradient is multivariate, too. It is a vector consisting of  $d$  partial derivatives:

$$\nabla f(\mathbf{x}) = \left[ \frac{\partial f(\mathbf{x})}{\partial x_1}, \frac{\partial f(\mathbf{x})}{\partial x_2}, \dots, \frac{\partial f(\mathbf{x})}{\partial x_d} \right]^\top. \quad (12.3.5)$$

Each partial derivative element  $\partial f(\mathbf{x})/\partial x_i$  in the gradient indicates the rate of change of  $f$  at  $\mathbf{x}$  with respect to the input  $x_i$ . As before in the univariate case we can use the corresponding Taylor approximation for multivariate functions to get some idea of what we should do. In particular, we have that

$$f(\mathbf{x} + \epsilon) = f(\mathbf{x}) + \epsilon^\top \nabla f(\mathbf{x}) + O(\|\epsilon\|^2). \quad (12.3.6)$$

In other words, up to second order terms in `epsilon` the direction of steepest descent is given by the negative gradient  $-\nabla f(\mathbf{x})$ . Choosing a suitable learning rate  $\eta > 0$  yields the prototypical gradient descent algorithm:

$$\mathbf{x} \leftarrow \mathbf{x} - \eta \nabla f(\mathbf{x}).$$

To see how the algorithm behaves in practice let's construct an objective function  $f(\mathbf{x}) = x_1^2 + 2x_2^2$  with a two-dimensional vector  $\mathbf{x} = [x_1, x_2]^\top$  as input and a scalar as output. The gradient is given by  $\nabla f(\mathbf{x}) = [2x_1, 4x_2]^\top$ . We will observe the trajectory of  $\mathbf{x}$  by gradient descent from the initial position  $[-5, -2]$ . We need two more helper functions. The first uses an update function and applies it 20 times to the initial value. The second helper visualizes the trajectory of  $\mathbf{x}$ .

```
# Save to the d2l package.
def train_2d(trainer):
    """Optimize a 2-dim objective function with a customized trainer."""
    # s1 and s2 are internal state variables and will
    # be used later in the chapter
    x1, x2, s1, s2 = -5, -2, 0, 0
    results = [(x1, x2)]
    for i in range(20):
        x1, x2, s1, s2 = trainer(x1, x2, s1, s2)
        results.append((x1, x2))
    return results
```

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```

x1, x2, s1, s2 = trainer(x1, x2, s1, s2)
    results.append((x1, x2))
print('epoch %d, x1 %f, x2 %f' % (i + 1, x1, x2))
return results

# Save to the d2l package.
def show_trace_2d(f, results):
    """Show the trace of 2D variables during optimization."""
    d2l.set_figsize((3.5, 2.5))
    d2l.plt.plot(*zip(*results), '-o', color='#ff7f0e')
    x1, x2 = np.meshgrid(np.arange(-5.5, 1.0, 0.1), np.arange(-3.0, 1.0, 0.1))
    d2l.plt.contour(x1, x2, f(x1, x2), colors='#1f77b4')
    d2l.plt.xlabel('x1')
    d2l.plt.ylabel('x2')

```

Next, we observe the trajectory of the optimization variable  $\mathbf{x}$  for learning rate  $\eta = 0.1$ . We can see that after 20 steps the value of  $\mathbf{x}$  approaches its minimum at  $[0, 0]$ . Progress is fairly well-behaved albeit rather slow.

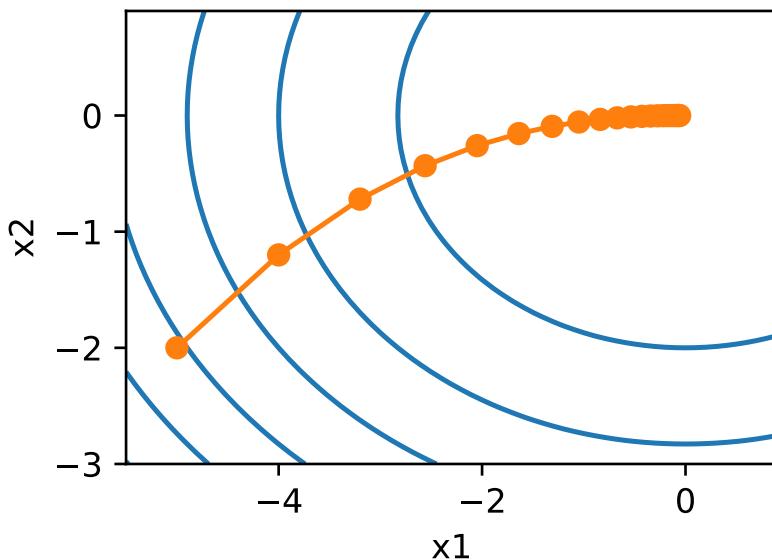
```

def f(x1, x2): return x1 ** 2 + 2 * x2 ** 2    # objective
def gradf(x1, x2): return (2 * x1, 4 * x2)      # gradient
def gd(x1, x2, s1, s2):
    (g1, g2) = gradf(x1, x2)                      # compute gradient
    return (x1 - eta * g1, x2 - eta * g2, 0, 0)   # update variables

eta = 0.1
show_trace_2d(f, train_2d(gd))

```

```
epoch 20, x1 -0.057646, x2 -0.000073
```



### 12.3.3 Adaptive Methods

As we could see in [Section 12.3.1](#), getting the learning rate  $\eta$  ‘just right’ is tricky. If we pick it too small, we make no progress. If we pick it too large, the solution oscillates and in the worst case it might even diverge. What if we could determine  $\eta$  automatically or get rid of having to select a step size at all? Second order methods that look not only at the value and gradient of the objective but also at its *curvature* can help in this case. While these methods cannot be applied to deep learning directly due to the computational cost, they provide useful intuition into how to design advanced optimization algorithms that mimic many of the desirable properties of the algorithms outlined below.

#### Newton’s Method

Reviewing the Taylor expansion of  $f$  there’s no need to stop after the first term. In fact, we can write it as

$$f(\mathbf{x} + \epsilon) = f(\mathbf{x}) + \epsilon^\top \nabla f(\mathbf{x}) + \frac{1}{2} \epsilon^\top \nabla \nabla^\top f(\mathbf{x}) \epsilon + O(\|\epsilon\|^3) \quad (12.3.7)$$

To avoid cumbersome notation we define  $H_f := \nabla \nabla^\top f(\mathbf{x})$  to be the *Hessian* of  $f$ . This is a  $d \times d$  matrix. For small  $d$  and simple problems  $H_f$  is easy to compute. For deep networks, on the other hand,  $H_f$  may be prohibitively large, due to the cost of storing  $O(d^2)$  entries. Furthermore it may be too expensive to compute via backprop as we would need to apply backprop to the backpropagation call graph. For now let us ignore such considerations and look at what algorithm we’d get.

After all, the minimum of  $f$  satisfies  $\nabla f(\mathbf{x}) = 0$ . Taking derivatives of (12.3.7) with regard to  $\epsilon$  and ignoring higher order terms we arrive at

$$\nabla f(\mathbf{x}) + H_f \epsilon = 0 \text{ and hence } \epsilon = -H_f^{-1} \nabla f(\mathbf{x}). \quad (12.3.8)$$

That is, we need to invert the Hessian  $H_f$  as part of the optimization problem.

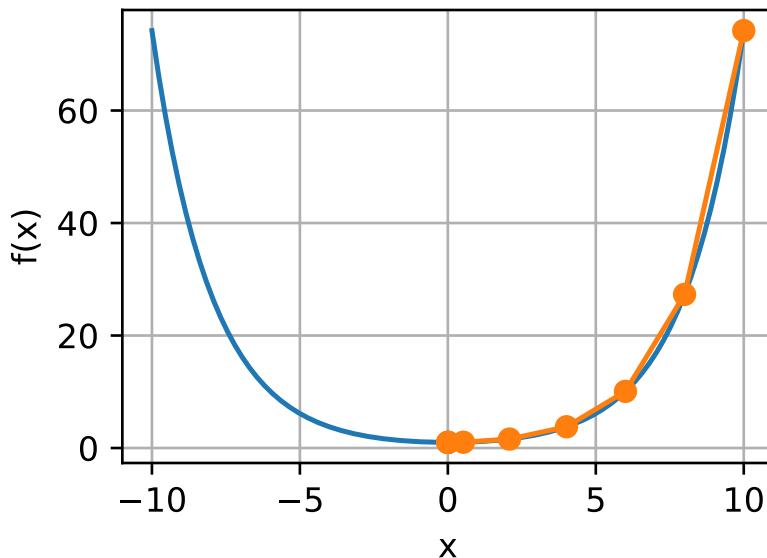
For  $f(x) = \frac{1}{2}x^2$  we have  $\nabla f(x) = x$  and  $H_f = 1$ . Hence for any  $x$  we obtain  $\epsilon = -x$ . In other words, a single step is sufficient to converge perfectly without the need for any adjustment! Alas, we got a bit lucky here since the Taylor expansion was exact. Let’s see what happens in other problems.

```
c = 0.5
def f(x):      return math.cosh(c * x)          # objective
def gradf(x):  return c * math.sinh(c * x)        # derivative
def hessf(x):  return c**2 * math.cosh(c * x) # hessian

# hide learning rate for now
def newton(eta = 1):
    x = 10
    results = [x]
    for i in range(10):
        x -= eta * gradf(x) / hessf(x)
        results.append(x)
    print('epoch 10, x:', x)
    return results

show_trace(newton())
```

```
epoch 10, x: 0.0
```

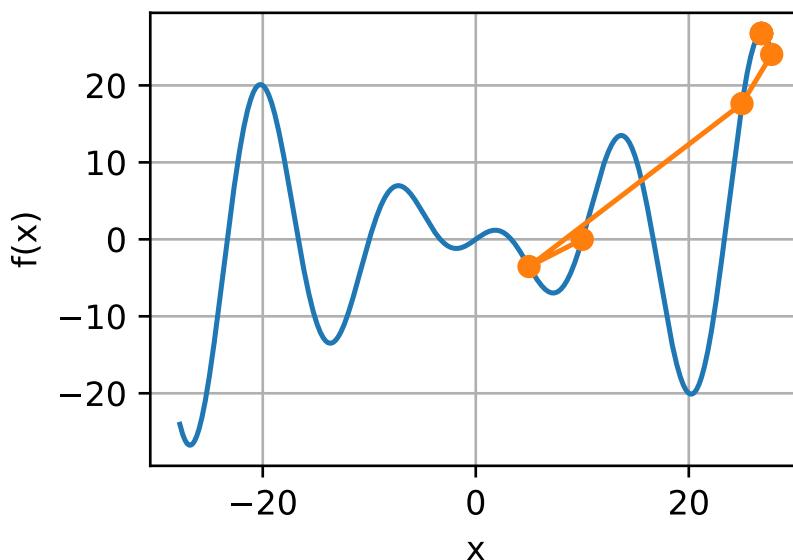


Now let's see what happens when we have a *nonconvex* function, such as  $f(x) = x \cos(cx)$ . After all, note that in Newton's method we end up dividing by the Hessian. This means that if the second derivative is *negative* we would walk into the direction of *increasing*  $f$ . That is a fatal flaw of the algorithm. Let's see what happens in practice.

```
c = 0.15 * math.pi
def f(x):      return x*math.cos(c * x)
def gradf(x):  return math.cos(c * x) - c * x * math.sin(c * x)
def hessf(x):  return - 2 * c * math.sin(c * x) - x * c**2 * math.cos(c * x)

show_trace(newton())
```

```
epoch 10, x: 26.83413291324767
```

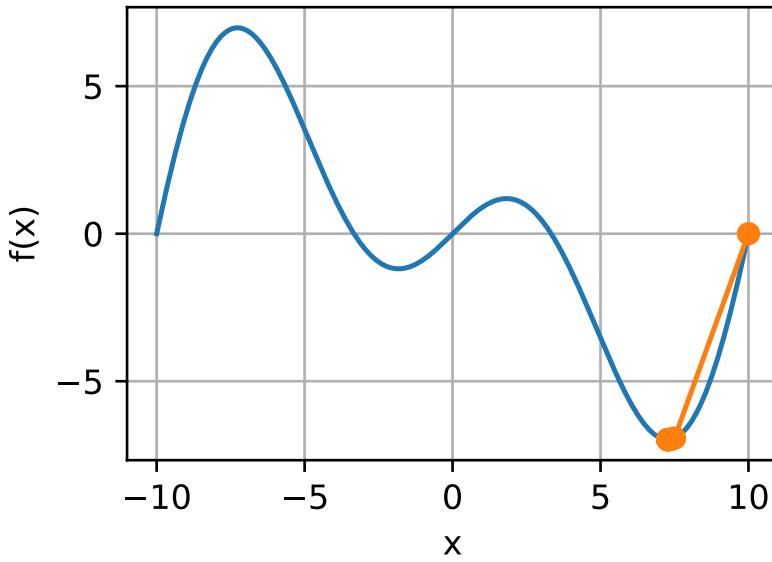


This went spectacularly wrong. How can we fix it? One way would be to 'fix' the Hessian by taking its

absolute value instead. Another strategy is to bring back the learning rate. This seems to defeat the purpose, but not quite. Having second order information allows us to be cautious whenever the curvature is large and to take longer steps whenever the objective is flat. Let's see how this works with a slightly smaller learning rate, say  $\eta = 0.5$ . As we can see, we have quite an efficient algorithm.

```
show_trace(newton(0.5))
```

```
epoch 10, x: 7.269860168684531
```



## Convergence Analysis

We only analyze the convergence rate for convex and three times differentiable  $f$ , where at its minimum  $x^*$  the second derivative is nonzero, i.e. where  $f''(x^*) > 0$ . The multivariate proof is a straightforward extension of the argument below and omitted since it doesn't help us much in terms of intuition.

Denote by  $x_k$  the value of  $x$  at the  $k$ -th iteration and let  $e_k := x_k - x^*$  be the distance from optimality. By Taylor series expansion we have that the condition  $f'(x^*) = 0$  can be written as

$$0 = f'(x_k - e_k) = f'(x_k) - e_k f''(x_k) + \frac{1}{2} e_k^2 f'''(\xi_k). \quad (12.3.9)$$

This holds for some  $\xi_k \in [x_k - e_k, x_k]$ . Recall that we have the update  $x_{k+1} = x_k - f'(x_k)/f''(x_k)$ . Dividing the above expansion by  $f''(x_k)$  yields

$$e_k - f'(x_k)/f''(x_k) = \frac{1}{2} e_k^2 f'''(\xi_k)/f'(x_k) \quad (12.3.10)$$

Plugging in the update equations leads to the following bound  $e_{k+1} \leq e_k^2 f'''(\xi_k)/f'(x_k)$ . Consequently, whenever we are in a region of bounded  $f'''(\xi_k)/f'(x_k) \leq c$ , we have a quadratically decreasing error  $e_{k+1} \leq c e_k^2$ .

As an aside, optimization researchers call this *linear* convergence, whereas a condition such as  $e_{k+1} \leq \alpha e_k$  would be called a *constant* rate of convergence. Note that this analysis comes with a number of caveats: We don't really have much of a guarantee when we will reach the region of rapid convergence. Instead, we only know that once we reach it, convergence will be very quick. Second, this requires that  $f$  is well-behaved up to higher order derivatives. It comes down to ensuring that  $f$  doesn't have any 'surprising' properties in terms of how it might change its values.

## Preconditioning

Quite unsurprisingly computing and storing the full Hessian is very expensive. It is thus desirable to find alternatives. One way to improve matters is by avoiding to compute the Hessian in its entirety but only compute the *diagonal* entries. While this isn't quite as good as the full Newton method, it is still much better than not using it. Moreover, estimates for the main diagonal elements are what drives some of the innovation in stochastic gradient descent optimization algorithms. This leads to update algorithms of the form

$$\mathbf{x} \leftarrow \mathbf{x} - \eta \text{diag}(H_f)^{-1} \nabla \mathbf{x}. \quad (12.3.11)$$

To see why this might be a good idea consider a situation where one variable denotes height in millimeters and the other one denotes height in kilometers. Assuming that for both the natural scale is in meters we have a terrible mismatch in parametrizations. Using preconditioning removes this. Effectively preconditioning with gradient descent amounts to selecting a different learning rate for each coordinate.

## Gradient Descent with Line Search

One of the key problems in gradient descent was that we might overshoot the goal or make insufficient progress. A simple fix for the problem is to use line search in conjunction with gradient descent. That is, we use the direction given by  $\nabla f(\mathbf{x})$  and then perform binary search as to which steplength  $\eta$  minimizes  $f(x - \eta \nabla f(\mathbf{x}))$ .

This algorithm converges rapidly (for an analysis and proof see e.g. [6]). However, for the purpose of deep learning this isn't quite so feasible, since each step of the line search would require us to evaluate the objective function on the entire dataset. This is way too costly to accomplish.

### 12.3.4 Summary

- Learning rates matter. Too large and we diverge, too small and we don't make progress.
- Gradient descent can get stuck in local minima.
- In high dimensions adjusting learning the learning rate is complicated.
- Preconditioning can help with scale adjustment.
- Newton's method is a lot faster *once* it has started working properly in convex problems.
- Beware of using Newton's method without any adjustments for nonconvex problems.

### 12.3.5 Exercises

1. Experiment with different learning rates and objective functions for gradient descent.
2. Implement line search to minimize a convex function in the interval  $[a, b]$ .
  - Do you need derivatives for binary search, i.e. to decide whether to pick  $[a, (a+b)/2]$  or  $[(a+b)/2, b]$ .
  - How rapid is the rate of convergence for the algorithm?
  - Implement the algorithm and apply it to minimizing  $\log(\exp(x) + \exp(-2 * x - 3))$ .
3. Design an objective function defined on  $\mathbb{R}^2$  where gradient descent is exceedingly slow. Hint - scale different coordinates differently.
4. Implement the lightweight version of Newton's method using preconditioning:

- Use diagonal Hessian as preconditioner.
  - Use the absolute values of that rather than the actual (possibly signed) values.
  - Apply this to the problem above.
5. Apply the algorithm above to a number of objective functions (convex or not). What happens if you rotate coordinates by 45 degrees?

### 12.3.6 Scan the QR Code to Discuss<sup>162</sup>



## 12.4 Stochastic Gradient Descent

In this section, we are going to introduce the basic principles of stochastic gradient descent.

```
%matplotlib inline
import d2l
import math
import numpy as np
```

Next, we use  $x = 10$  as the initial value and assume  $\eta = 0.2$ . Using gradient descent to iterate  $x$  10 times, we can see that, eventually, the value of  $x$  approaches the optimal solution.

### 12.4.1 Stochastic Gradient Descent (SGD)

In deep learning, the objective function is usually the average of the loss functions for each example in the training data set. We assume that  $f_i(\mathbf{x})$  is the loss function of the training data instance with  $n$  examples, an index of  $i$ , and parameter vector of  $\mathbf{x}$ , then we have the objective function

$$f(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n f_i(\mathbf{x}). \quad (12.4.1)$$

The gradient of the objective function at  $\mathbf{x}$  is computed as

$$\nabla f(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \nabla f_i(\mathbf{x}). \quad (12.4.2)$$

If gradient descent is used, the computing cost for each independent variable iteration is  $\mathcal{O}(n)$ , which grows linearly with  $n$ . Therefore, when the model training data instance is large, the cost of gradient descent for each iteration will be very high.

Stochastic gradient descent (SGD) reduces computational cost at each iteration. At each iteration of stochastic gradient descent, we uniformly sample an index  $i \in \{1, \dots, n\}$  for data instances at random, and compute

<sup>162</sup> <https://discuss.mxnet.io/t/2372>

the gradient  $\nabla f_i(\mathbf{x})$  to update  $\mathbf{x}$ :

$$\mathbf{x} \leftarrow \mathbf{x} - \eta \nabla f_i(\mathbf{x}). \quad (12.4.3)$$

Here,  $\eta$  is the learning rate. We can see that the computing cost for each iteration drops from  $\mathcal{O}(n)$  of the gradient descent to the constant  $\mathcal{O}(1)$ . We should mention that the stochastic gradient  $\nabla f_i(\mathbf{x})$  is the unbiased estimate of gradient  $\nabla f(\mathbf{x})$ .

$$\mathbb{E}_i \nabla f_i(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \nabla f_i(\mathbf{x}) = \nabla f(\mathbf{x}). \quad (12.4.4)$$

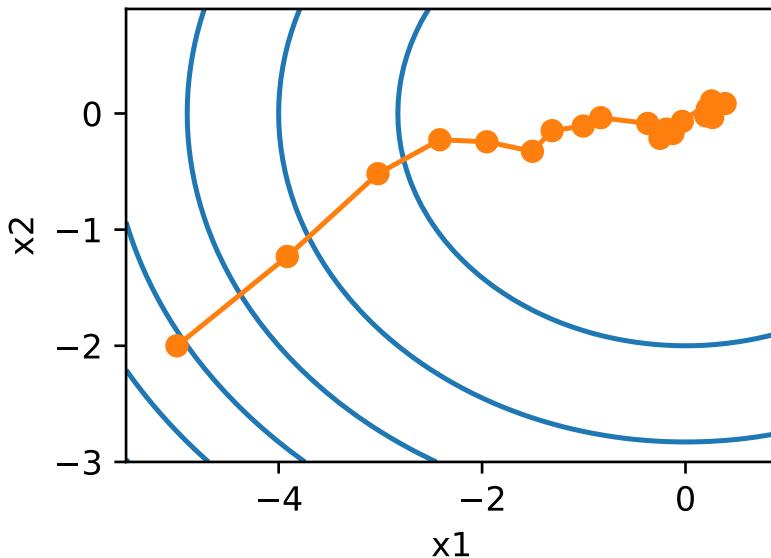
This means that, on average, the stochastic gradient is a good estimate of the gradient.

Now, we will compare it to gradient descent by adding random noise with a mean of 0 to the gradient to simulate a SGD.

```
def f(x1, x2): return x1 ** 2 + 2 * x2 ** 2      # objective
def gradf(x1, x2): return (2 * x1, 4 * x2)        # gradient
def sgd(x1, x2, s1, s2):                          # simulate noisy gradient
    (g1, g2) = gradf(x1, x2)                      # compute gradient
    (g1, g2) = (g1 + np.random.normal(0.1), g2 + np.random.normal(0.1))
    return (x1 - eta * g1, x2 - eta * g2, 0, 0)   # update variables

eta = 0.1
d2l.show_trace_2d(f, d2l.train_2d(sgd))
```

```
epoch 20, x1 0.247942, x2 0.038134
```



As we can see, the iterative trajectory of the independent variable in the SGD is more tortuous than in the gradient descent. This is due to the noise added in the experiment, which reduced the accuracy of the simulated stochastic gradient. In practice, such noise usually comes from individual examples in the training data set.

### 12.4.2 Summary

- If we use a more suitable learning rate and update the independent variable in the opposite direction of the gradient, the value of the objective function might be reduced. Gradient descent repeats this update process until a solution that meets the requirements is obtained.
- Problems occur when the learning rate is too small or too large. A suitable learning rate is usually found only after multiple experiments.
- When there are more examples in the training data set, it costs more to compute each iteration for gradient descent, so SGD is preferred in these cases.

### 12.4.3 Exercises

- Using a different objective function, observe the iterative trajectory of the independent variable in gradient descent and the SGD.
- In the experiment for gradient descent in two-dimensional space, try to use different learning rates to observe and analyze the experimental phenomena.

### 12.4.4 Scan the QR Code to Discuss<sup>163</sup>



## 12.5 Mini-batch Stochastic Gradient Descent

In each iteration, the gradient descent uses the entire training data set to compute the gradient, so it is sometimes referred to as batch gradient descent. Stochastic gradient descent (SGD) only randomly select one example in each iteration to compute the gradient. Just like in the previous chapters, we can perform random uniform sampling for each iteration to form a mini-batch and then use this mini-batch to compute the gradient. Now, we are going to discuss mini-batch stochastic gradient descent.

Set objective function  $f(\mathbf{x}) : \mathbb{R}^d \rightarrow \mathbb{R}$ . The time step before the start of iteration is set to 0. The independent variable of this time step is  $\mathbf{x}_0 \in \mathbb{R}^d$  and is usually obtained by random initialization. In each subsequent time step  $t > 0$ , mini-batch SGD uses random uniform sampling to get a mini-batch  $\mathcal{B}_t$  made of example indices from the training data set. We can use sampling with replacement or sampling without replacement to get a mini-batch example. The former method allows duplicate examples in the same mini-batch, the latter does not and is more commonly used. We can use either of the two methods

$$\mathbf{g}_t \leftarrow \nabla f_{\mathcal{B}_t}(\mathbf{x}_{t-1}) = \frac{1}{|\mathcal{B}|} \sum_{i \in \mathcal{B}_t} \nabla f_i(\mathbf{x}_{t-1}) \quad (12.5.1)$$

to compute the gradient  $\mathbf{g}_t$  of the objective function at  $\mathbf{x}_{t-1}$  with mini-batch  $\mathcal{B}_t$  at time step  $t$ . Here,  $|\mathcal{B}|$  is the size of the batch, which is the number of examples in the mini-batch. This is a hyper-parameter. Just like the stochastic gradient, the mini-batch SGD  $\mathbf{g}_t$  obtained by sampling with replacement is also the unbiased

<sup>163</sup> <https://discuss.mxnet.io/t/2372>

estimate of the gradient  $\nabla f(\mathbf{x}_{t-1})$ . Given the learning rate  $\eta_t$  (positive), the iteration of the mini-batch SGD on the independent variable is as follows:

$$\mathbf{x}_t \leftarrow \mathbf{x}_{t-1} - \eta_t \mathbf{g}_t. \quad (12.5.2)$$

The variance of the gradient based on random sampling cannot be reduced during the iterative process, so in practice, the learning rate of the (mini-batch) SGD can self-decay during the iteration, such as  $\eta_t = \eta t^\alpha$  (usually  $\alpha = -1$  or  $-0.5$ ),  $\eta_t = \eta \alpha^t$  (e.g  $\alpha = 0.95$ ), or learning rate decay once per iteration or after several iterations. As a result, the variance of the learning rate and the (mini-batch) SGD will decrease. Gradient descent always uses the true gradient of the objective function during the iteration, without the need to self-decay the learning rate.

The cost for computing each iteration is  $\mathcal{O}(|\mathcal{B}|)$ . When the batch size is 1, the algorithm is an SGD; when the batch size equals the example size of the training data, the algorithm is a gradient descent. When the batch size is small, fewer examples are used in each iteration, which will result in parallel processing and reduce the RAM usage efficiency. This makes it more time consuming to compute examples of the same size than using larger batches. When the batch size increases, each mini-batch gradient may contain more redundant information. To get a better solution, we need to compute more examples for a larger batch size, such as increasing the number of epochs.

### 12.5.1 Reading Data

In this chapter, we will use a data set<sup>164</sup> developed by NASA to test the wing noise from different aircraft to compare these optimization algorithms. We will use the first 1500 examples of the data set, 5 features, and a normalization method to preprocess the data.

```
%matplotlib inline
import d2l
from mxnet import autograd, gluon, init, nd
from mxnet.gluon import nn
import numpy as np

# Save to the d2l package.
def get_data_ch10(batch_size=10, n=1500):
    data = np.genfromtxt('../data/airfoil_self_noise.dat', delimiter='\t')
    data = nd.array((data - data.mean(axis=0)) / data.std(axis=0))
    data_iter = d2l.load_array((data[:n, :-1], data[:n, -1]),
                               batch_size, is_train=True)
    return data_iter, data.shape[1]-1
```

### 12.5.2 Implementation from Scratch

We have already implemented the mini-batch SGD algorithm in the Section 5.2. We have made its input parameters more generic here, so that we can conveniently use the same input for the other optimization algorithms introduced later in this chapter. Specifically, we add the status input `states` and place the hyper-parameter in dictionary `hyperparams`. In addition, we will average the loss of each mini-batch example in the training function, so the gradient in the optimization algorithm does not need to be divided by the batch size.

---

<sup>164</sup> <https://archive.ics.uci.edu/ml/datasets/Airfoil+Self-Noise>

```
def sgd(params, states, hyperparams):
    for p in params:
        p[:] -= hyperparams['lr'] * p.grad
```

Next, we are going to implement a generic training function to facilitate the use of the other optimization algorithms introduced later in this chapter. It initializes a linear regression model and can then be used to train the model with the mini-batch SGD and other algorithms introduced in subsequent sections.

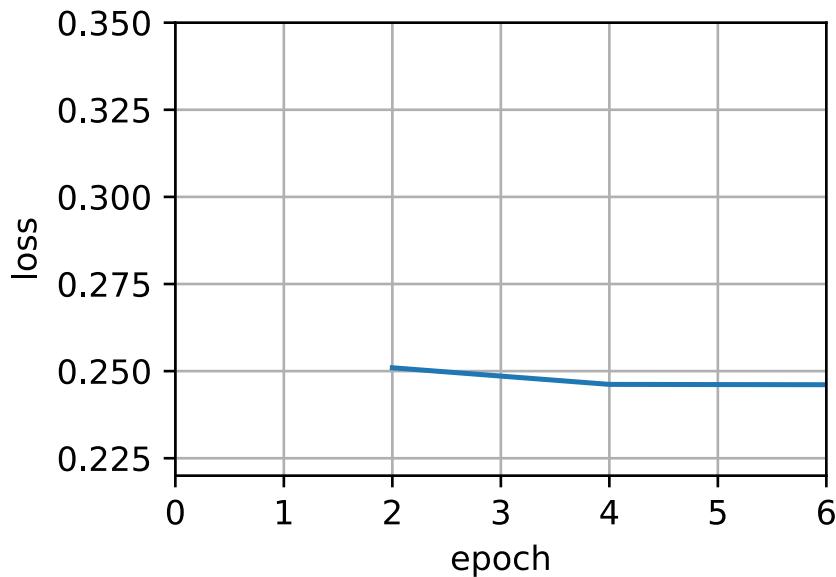
```
# Save to the d2l package.
def train_ch10(trainer_fn, states, hyperparams, data_iter,
               feature_dim, num_epochs=2):
    # Initialization
    w = nd.random.normal(scale=0.01, shape=(feature_dim, 1))
    b = nd.zeros(1)
    w.attach_grad()
    b.attach_grad()
    net, loss = lambda X: d2l.linreg(X, w, b), d2l.squared_loss
    # Train
    animator = d2l.Animator(xlabel='epoch', ylabel='loss',
                             xlim=[0, num_epochs], ylim=[0.22, 0.35])
    n, timer = 0, d2l.Timer()
    for _ in range(num_epochs):
        for X, y in data_iter:
            with autograd.record():
                l = loss(net(X), y).mean()
            l.backward()
            trainer_fn([w, b], states, hyperparams)
            n += X.shape[0]
            if n % 200 == 0:
                timer.stop()
                animator.add(n/X.shape[0]/len(data_iter),
                             d2l.evaluate_loss(net, data_iter, loss))
                timer.start()
        print('loss: %.3f, %.3f sec/epoch'%(animator.Y[0][-1], timer.avg()))
    return timer.cumsum(), animator.Y[0]
```

When the batch size equals 1500 (the total number of examples), we use gradient descent for optimization. The model parameters will be iterated only once for each epoch of the gradient descent. As we can see, the downward trend of the value of the objective function (training loss) flattened out after 6 iterations.

```
def train_sgd(lr, batch_size, num_epochs=2):
    data_iter, feature_dim = get_data_ch10(batch_size)
    return train_ch10(
        sgd, None, {'lr': lr}, data_iter, feature_dim, num_epochs)

gd_res = train_sgd(1, 1500, 6)
```

```
loss: 0.246, 0.048 sec/epoch
```

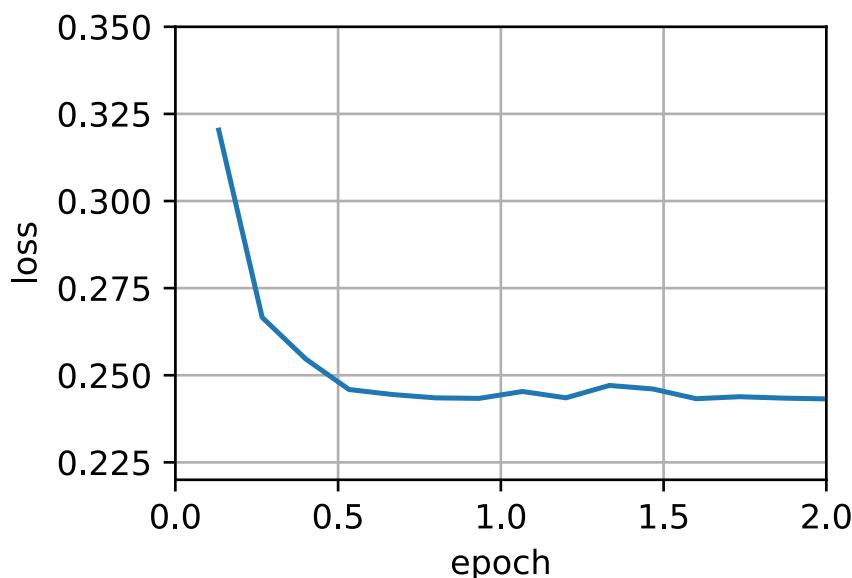


When the batch size equals 1, we use SGD for optimization. In order to simplify the implementation, we did not self-decay the learning rate. Instead, we simply used a small constant for the learning rate in the (mini-batch) SGD experiment. In SGD, the independent variable (model parameter) is updated whenever an example is processed. Thus it is updated 1500 times in one epoch. As we can see, the decline in the value of the objective function slows down after one epoch.

Although both the procedures processed 1500 examples within one epoch, SGD consumes more time than gradient descent in our experiment. This is because SGD performed more iterations on the independent variable within one epoch, and it is harder for single-example gradient computation to use parallel computing effectively.

```
sgd_res = train_sgd(0.005, 1)
```

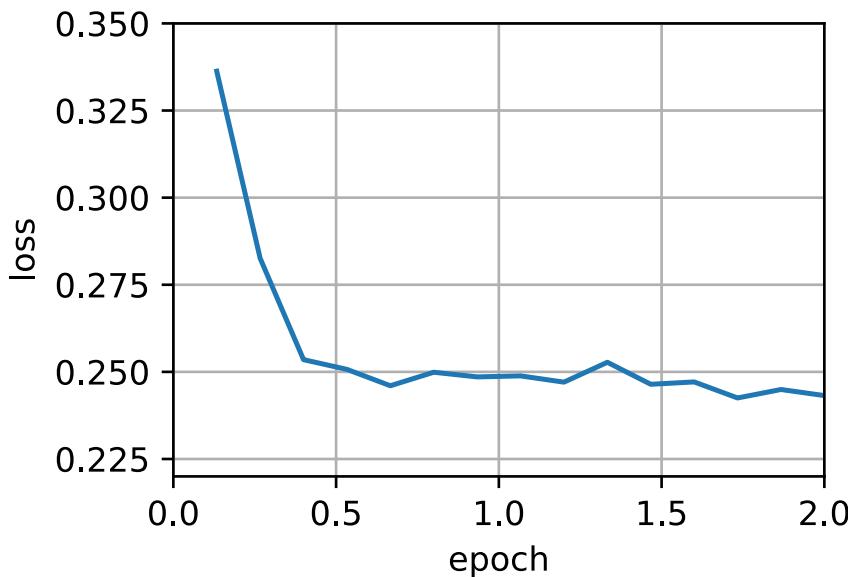
```
loss: 0.243, 0.291 sec/epoch
```



When the batch size equals 100, we use mini-batch SGD for optimization. The time required for one epoch is between the time needed for gradient descent and SGD to complete the same epoch.

```
mini1_res = train_sgd(.4, 100)
```

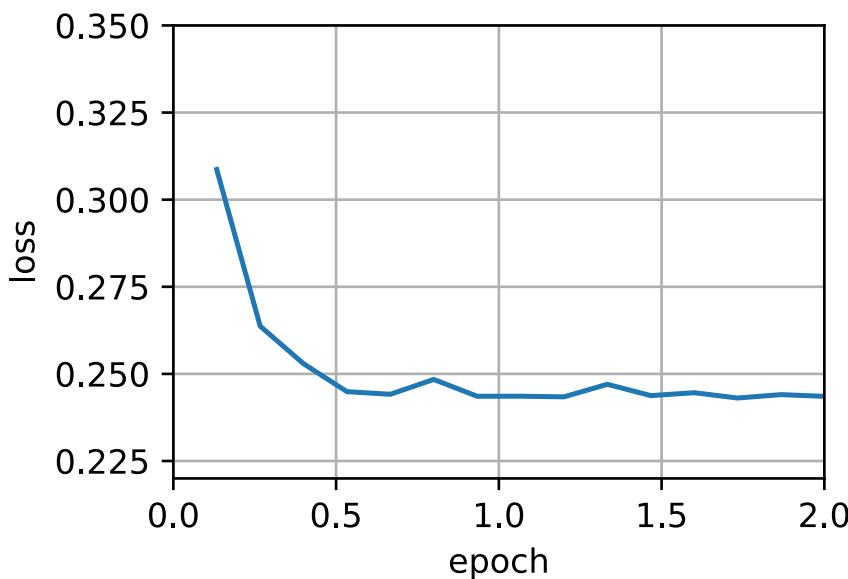
```
loss: 0.243, 0.007 sec/epoch
```



Reduce the batch size to 10, the time for each epoch increases because the workload for each batch is less efficient to execute.

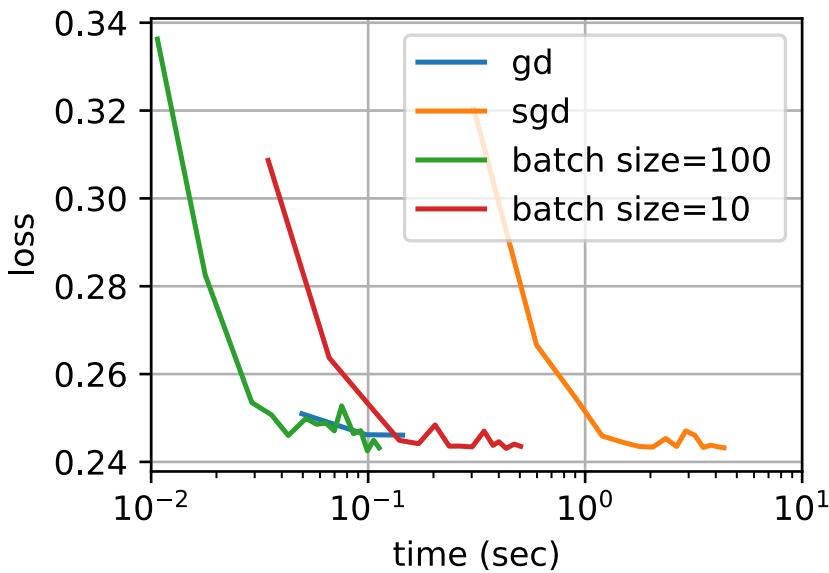
```
mini2_res = train_sgd(.05, 10)
```

```
loss: 0.244, 0.034 sec/epoch
```



Finally, we compare the time versus loss for the previous four experiments. As can be seen, despite SGD converges faster than GD in terms of number of examples processed, it uses more time to reach the same loss than GD because that computing gradient example by example is not efficient. Mini-batch SGD is able to trade-off the convergence speed and computation efficiency. Here, a batch size 10 improves SGD, and a batch size 100 even outperforms GD.

```
d2l.set_figsize([6, 3])
d2l.plot(*list(map(list, zip(gd_res, sgd_res, mini1_res, mini2_res))),
         'time (sec)', 'loss', xlim=[1e-2, 10],
         legend=['gd', 'sgd', 'batch size=100', 'batch size=10'])
d2l.plt.gca().set_xscale('log')
```



### 12.5.3 Concise Implementation

In Gluon, we can use the `Trainer` class to call optimization algorithms. Next, we are going to implement a generic training function that uses the optimization name `trainer_name` and hyperparameter `trainer_hyperparameter` to create the instance `Trainer`.

```
# Save to the d2l package.
def train_gluon_ch10(trainer_name, trainer_hyperparams,
                     data_iter, num_epochs=2):
    # Initialization
    net = nn.Sequential()
    net.add(nn.Dense(1))
    net.initialize(init.Normal(sigma=0.01))
    trainer = gluon.Trainer(
        net.collect_params(), trainer_name, trainer_hyperparams)
    loss = gluon.loss.L2Loss()
    animator = d2l.Animator(xlabel='epoch', ylabel='loss',
                           xlim=[0, num_epochs], ylim=[0.22, 0.35])
    n, timer = 0, d2l.Timer()
    for _ in range(num_epochs):
```

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```

for X, y in data_iter:
    with autograd.record():
        l = loss(net(X), y)
    l.backward()
    trainer.step(X.shape[0])
    n += X.shape[0]
    if n % 200 == 0:
        timer.stop()
        animator.add(n/X.shape[0]/len(data_iter),
                     d2l.evaluate_loss(net, data_iter, loss))
        timer.start()
print('loss: %.3f, %.3f sec/epoch'%(animator.Y[0][-1], timer.avg()))

```

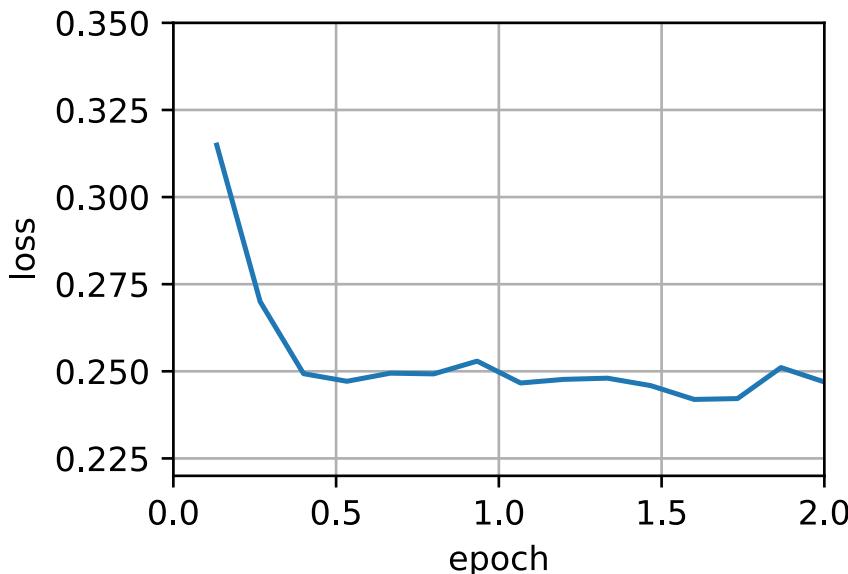
Use Gluon to repeat the last experiment.

```

data_iter, _ = get_data_ch10(10)
train_gluon_ch10('sgd', {'learning_rate': 0.05}, data_iter)

```

```
loss: 0.247, 0.033 sec/epoch
```



#### 12.5.4 Summary

- Mini-batch stochastic gradient uses random uniform sampling to get a mini-batch training example for gradient computation.
- In practice, learning rates of the (mini-batch) SGD can self-decay during iteration.
- In general, the time consumption per epoch for mini-batch stochastic gradient is between what takes for gradient descent and SGD to complete the same epoch.

### 12.5.5 Exercises

- Modify the batch size and learning rate and observe the rate of decline for the value of the objective function and the time consumed in each epoch.
- Read the MXNet documentation and use the Trainer class `set_learning_rate` function to reduce the learning rate of the mini-batch SGD to 1/10 of its previous value after each epoch.

### 12.5.6 Scan the QR Code to Discuss<sup>165</sup>



## 12.6 Momentum

In Section 12.3, we mentioned that the gradient of the objective function's independent variable represents the direction of the objective function's fastest descend at the current position of the independent variable. Therefore, gradient descent is also called steepest descent. In each iteration, the gradient descends according to the current position of the independent variable while updating the latter along the current position of the gradient. However, this can lead to problems if the iterative direction of the independent variable relies exclusively on the current position of the independent variable.

### 12.6.1 Exercises with Gradient Descent

Now, we will consider an objective function  $f(\mathbf{x}) = 0.1x_1^2 + 2x_2^2$ , whose input and output are a two-dimensional vector  $\mathbf{x} = [x_1, x_2]$  and a scalar, respectively. In contrast to Section 12.3, here, the coefficient  $x_1^2$  is reduced from 1 to 0.1. We are going to implement gradient descent based on this objective function, and demonstrate the iterative trajectory of the independent variable using the learning rate 0.4.

```
%matplotlib inline
import d2l
from mxnet import nd

eta = 0.4

def f_2d(x1, x2):
    return 0.1 * x1 ** 2 + 2 * x2 ** 2

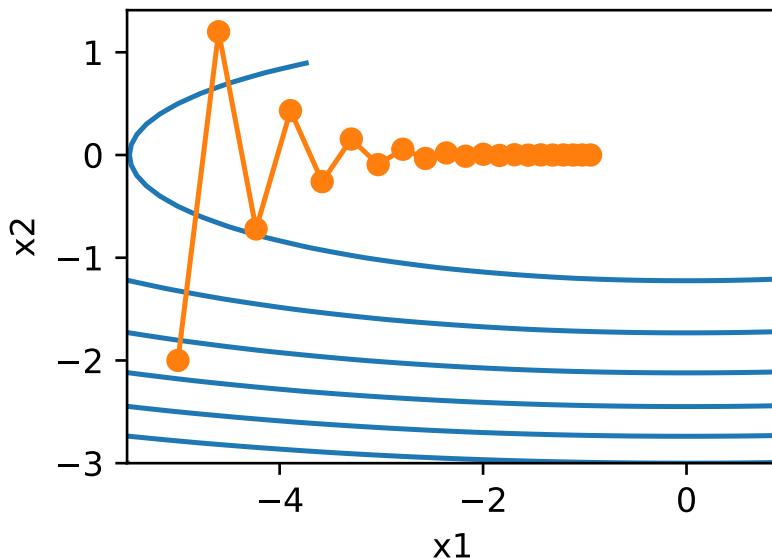
def gd_2d(x1, x2, s1, s2):
    return (x1 - eta * 0.2 * x1, x2 - eta * 4 * x2, 0, 0)

d2l.show_trace_2d(f_2d, d2l.train_2d(gd_2d))
```

---

<sup>165</sup> <https://discuss.mxnet.io/t/2373>

```
epoch 20, x1 -0.943467, x2 -0.000073
```

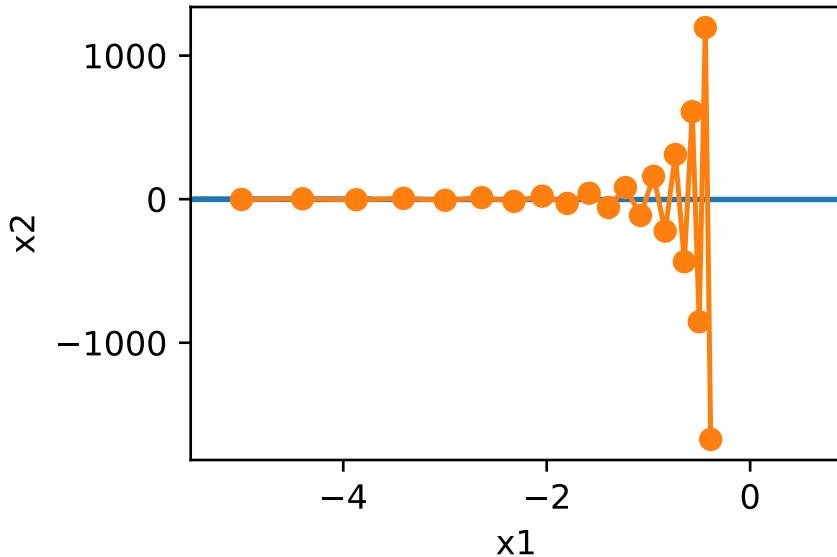


As we can see, at the same position, the slope of the objective function has a larger absolute value in the vertical direction ( $x_2$  axis direction) than in the horizontal direction ( $x_1$  axis direction). Therefore, given the learning rate, using gradient descent for interaction will cause the independent variable to move more in the vertical direction than in the horizontal one. So we need a small learning rate to prevent the independent variable from overshooting the optimal solution for the objective function in the vertical direction. However, it will cause the independent variable to move slower toward the optimal solution in the horizontal direction.

Now, we try to make the learning rate slightly larger, so the independent variable will continuously overshoot the optimal solution in the vertical direction and gradually diverge.

```
eta = 0.6
d2l.show_trace_2d(f_2d, d2l.train_2d(gd_2d))
```

```
epoch 20, x1 -0.387814, x2 -1673.365109
```



## 12.6.2 The Momentum Method

The momentum method was proposed to solve the gradient descent problem described above. Since mini-batch stochastic gradient descent is more general than gradient descent, the subsequent discussion in this chapter will continue to use the definition for mini-batch stochastic gradient descent  $\mathbf{g}_t$  at time step  $t$  given in Section 12.5. We set the independent variable at time step  $t$  to  $\mathbf{x}_t$  and the learning rate to  $\eta_t$ . At time step 0, momentum creates the velocity variable  $\mathbf{v}_0$  and initializes its elements to zero. At time step  $t > 0$ , momentum modifies the steps of each iteration as follows:

$$\begin{aligned}\mathbf{v}_t &\leftarrow \gamma \mathbf{v}_{t-1} + \eta_t \mathbf{g}_t, \\ \mathbf{x}_t &\leftarrow \mathbf{x}_{t-1} - \mathbf{v}_t,\end{aligned}\tag{12.6.1}$$

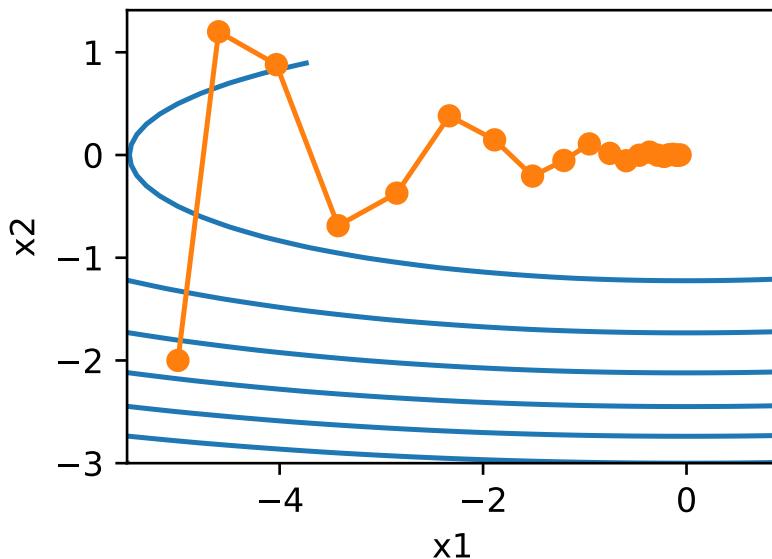
Here, the momentum hyperparameter  $\gamma$  satisfies  $0 \leq \gamma < 1$ . When  $\gamma = 0$ , momentum is equivalent to a mini-batch SGD.

Before explaining the mathematical principles behind the momentum method, we should take a look at the iterative trajectory of the gradient descent after using momentum in the experiment.

```
def momentum_2d(x1, x2, v1, v2):
    v1 = gamma * v1 + eta * 0.2 * x1
    v2 = gamma * v2 + eta * 4 * x2
    return x1 - v1, x2 - v2, v1, v2

eta, gamma = 0.4, 0.5
d2l.show_trace_2d(f_2d, d2l.train_2d(momentum_2d))
```

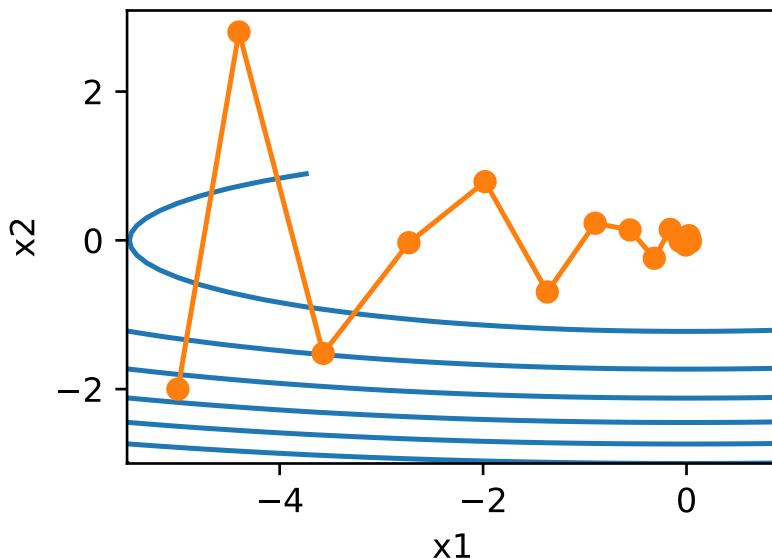
```
epoch 20, x1 -0.062843, x2 0.001202
```



As we can see, when using a smaller learning rate ( $\eta = 0.4$ ) and momentum hyperparameter ( $\gamma = 0.5$ ), momentum moves more smoothly in the vertical direction and approaches the optimal solution faster in the horizontal direction. Now, when we use a larger learning rate ( $\eta = 0.6$ ), the independent variable will no longer diverge.

```
eta = 0.6
d2l.show_trace_2d(f_2d, d2l.train_2d(momentum_2d))
```

```
epoch 20, x1 0.007188, x2 0.002553
```



### Expanding the velocity variable $\mathbf{v}_t$

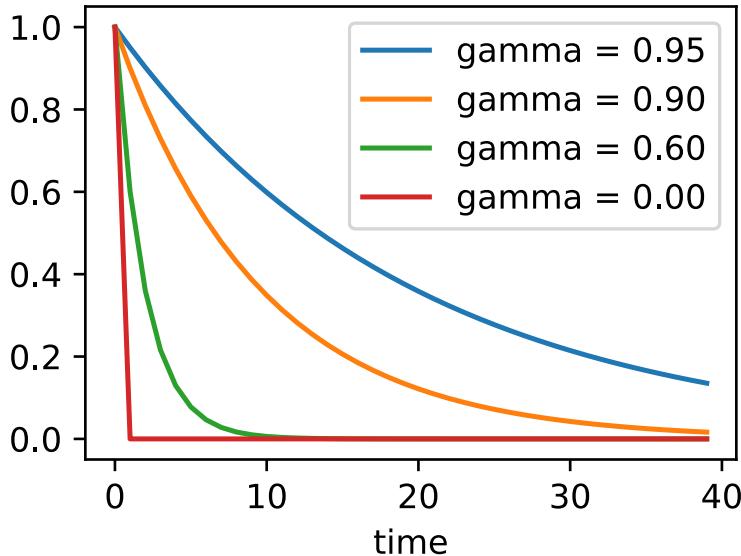
To understand the momentum method, we can expand the velocity variable over time:

$$\begin{aligned}\mathbf{v}_t &= \eta_t \mathbf{g}_t + \gamma \mathbf{v}_{t-1}, \\ &= \eta_t \mathbf{g}_t + \gamma \eta_{t-1} \mathbf{g}_{t-1} + \gamma \mathbf{v}_{t-1}, \\ &\dots \\ &= \eta_t \mathbf{g}_t + \gamma \eta_{t-1} \mathbf{g}_{t-1} + \dots + \gamma^{t-1} \eta_1 \mathbf{g}_1.\end{aligned}\tag{12.6.2}$$

As we can see that  $\mathbf{v}_t$  is a weighted sum over all past gradients multiplied by the according learning rate, which is the weight update in normal gradient descent. We just call it the scaled gradient. The weights deceases exponentially with the speed controlled by  $\gamma$ .

The following code block shows the weights for the past 40 time steps under various  $\gamma$ s.

```
gammas = [0.95, 0.9, 0.6, 0]
d2l.set_figsize((3.5, 2.5))
for gamma in gammas:
    x = nd.arange(40).asnumpy()
    d2l.plt.plot(x, gamma ** x, label='gamma = %.2f'%gamma)
d2l.plt.xlabel('time')
d2l.plt.legend();
```



A small  $\gamma$  will let the velocity variable focus on more recent scaled gradients. While a large value will have the velocity variable to include more past scaled gradients. Compared to the plain gradient descent, momentum will make the weight updates be more consistent over time. It might smooth the training progress if  $\mathbf{x}$  enters the region that the gradient vary, or walk out region that is too flat.

Also note that  $\frac{1}{1-\gamma} = 1 + \gamma + \gamma^2 + \dots$ . So all scaled gradients are similar to each other, e.g.  $\eta_t \mathbf{g}_t \approx \eta \mathbf{g}$  for all  $t$ s, then the momentum changes the weight updates from  $\eta \mathbf{g}$  in normal gradient descent into  $\frac{\eta}{1-\gamma} \mathbf{g}$ .

### 12.6.3 Implementation from Scratch

Compared with mini-batch SGD, the momentum method needs to maintain a velocity variable of the same shape for each independent variable and a momentum hyperparameter is added to the hyperparameter

category. In the implementation, we use the state variable `states` to represent the velocity variable in a more general sense.

```
def init_momentum_states(feature_dim):
    v_w = nd.zeros((feature_dim, 1))
    v_b = nd.zeros(1)
    return (v_w, v_b)

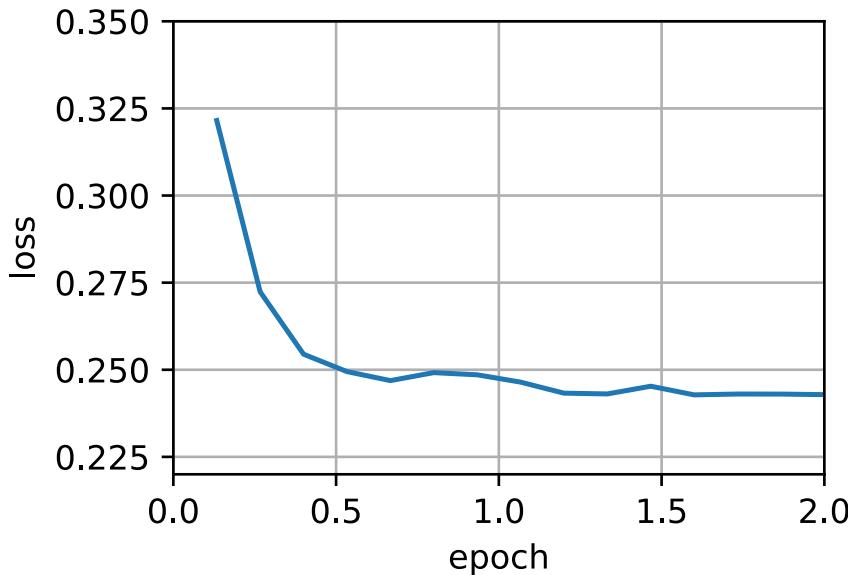
def sgd_momentum(params, states, hyperparams):
    for p, v in zip(params, states):
        v[:] = hyperparams['momentum'] * v + hyperparams['lr'] * p.grad
        p[:] -= v
```

When we set the momentum hyperparameter `momentum` to 0.5, it can be treated as a mini-batch SGD: the mini-batch gradient here is the weighted average of twice the mini-batch gradient of the last two time steps.

```
def train_momentum(lr, momentum, num_epochs=2):
    d2l.train_ch10(sgd_momentum, init_momentum_states(feature_dim),
                   {'lr': lr, 'momentum': momentum}, data_iter,
                   feature_dim, num_epochs)

data_iter, feature_dim = d2l.get_data_ch10(batch_size=10)
train_momentum(0.02, 0.5)
```

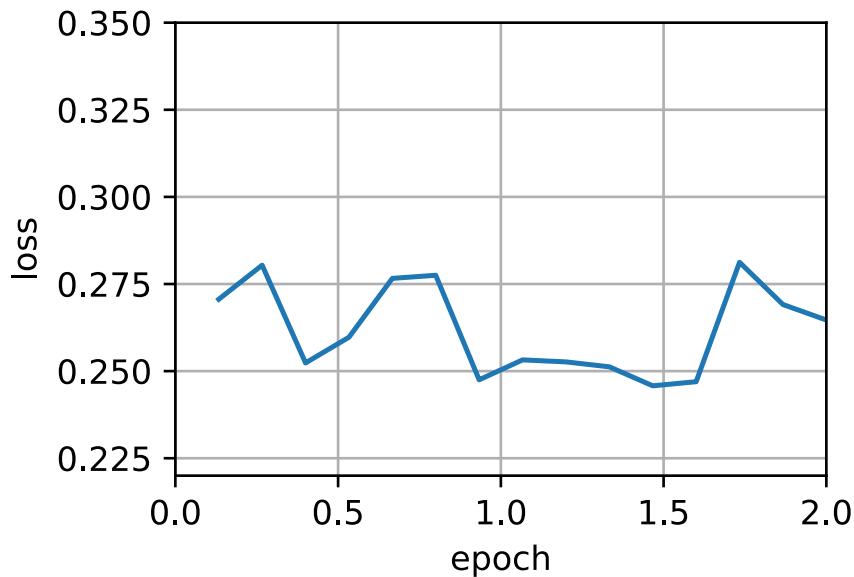
```
loss: 0.243, 0.037 sec/epoch
```



When we increase the momentum hyperparameter `momentum` to 0.9, it can still be treated as a mini-batch SGD: the mini-batch gradient here will be the weighted average of ten times the mini-batch gradient of the last 10 time steps. Now we keep the learning rate at 0.02.

```
train_momentum(0.02, 0.9)
```

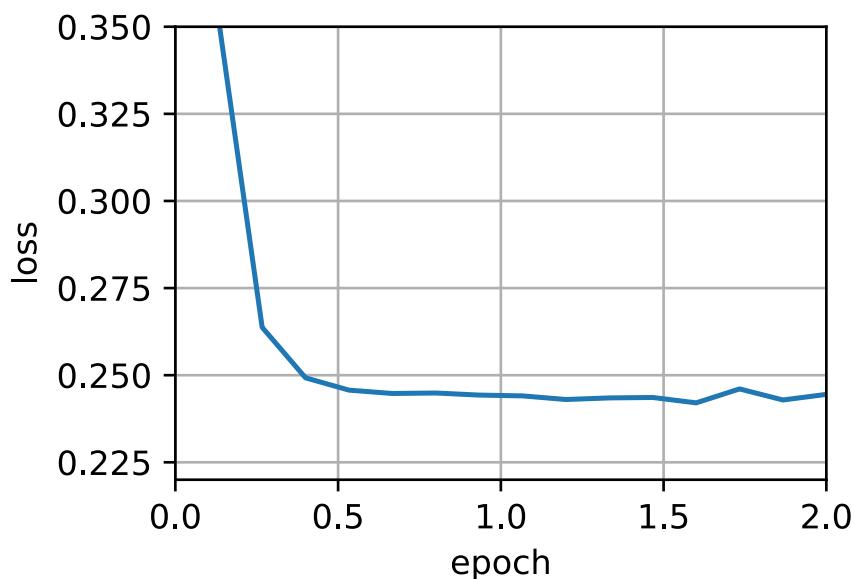
```
loss: 0.265, 0.037 sec/epoch
```



We can see that the value change of the objective function is not smooth enough at later stages of iteration. Intuitively, ten times the mini-batch gradient is five times larger than two times the mini-batch gradient, so we can try to reduce the learning rate to 1/5 of its original value. Now, the value change of the objective function becomes smoother after its period of decline.

```
train_momentum(0.004, 0.9)
```

```
loss: 0.244, 0.223 sec/epoch
```



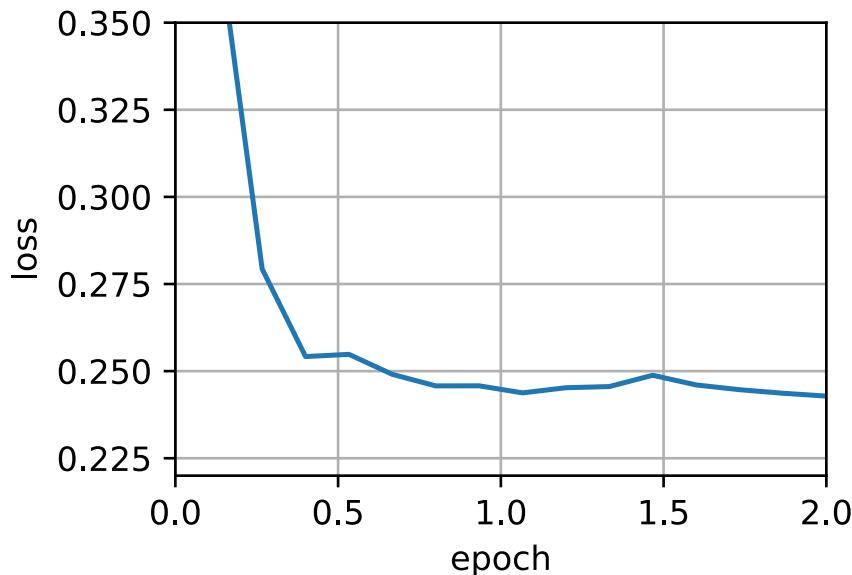
#### 12.6.4 Concise Implementation

In Gluon, we only need to use `momentum` to define the momentum hyperparameter in the `Trainer` instance to implement momentum.

```
d2l.train_gluon_ch10('sgd', {'learning_rate': 0.004, 'momentum': 0.9},  
    data_iter)
```

```
loss: 0.243, 0.199 sec/epoch
```

```
([0.17665648460388184,  
 0.23570585250854492,  
 0.43108248710632324,  
 0.7403717041015625,  
 0.8433592319488525,  
 1.0522971153259277,  
 1.1673743724822998,  
 1.2088489532470703,  
 1.6839773654937744,  
 1.8742008209228516,  
 2.110902786254883,  
 2.180490493774414,  
 2.6789679527282715,  
 2.7268285751342773,  
 2.9890730381011963],  
 [0.3728206636508306,  
 0.27933430206775667,  
 0.2541765211224556,  
 0.2548156104882558,  
 0.2490747149984042,  
 0.24575984686613084,  
 0.24578582696119944,  
 0.24375747621059418,  
 0.24523593155543008,  
 0.24556924911340078,  
 0.24881336802244186,  
 0.2460328230659167,  
 0.24467011618614196,  
 0.24364957318703334,  
 0.24283280193805695])
```



### 12.6.5 Summary

- The momentum method uses the EWMA concept. It takes the weighted average of past time steps, with weights that decay exponentially by the time step.
- Momentum makes independent variable updates for adjacent time steps more consistent in direction.

### 12.6.6 Exercises

- Use other combinations of momentum hyperparameters and learning rates and observe and analyze the different experimental results.

### 12.6.7 Scan the QR Code to Discuss<sup>166</sup>



## 12.7 Adagrad

In the optimization algorithms we introduced previously, each element of the objective function's independent variables uses the same learning rate at the same time step for self-iteration. For example, if we assume that the objective function is  $f$  and the independent variable is a two-dimensional vector  $[x_1, x_2]^\top$ , each element

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<sup>166</sup> <https://discuss.mxnet.io/t/2374>

in the vector uses the same learning rate when iterating. For example, in gradient descent with the learning rate  $\eta$ , element  $x_1$  and  $x_2$  both use the same learning rate  $\eta$  for iteration:

$$x_1 \leftarrow x_1 - \eta \frac{\partial f}{\partial x_1}, \quad x_2 \leftarrow x_2 - \eta \frac{\partial f}{\partial x_2}. \quad (12.7.1)$$

In Section 12.6, we can see that, when there is a big difference between the gradient values  $x_1$  and  $x_2$ , a sufficiently small learning rate needs to be selected so that the independent variable will not diverge in the dimension of larger gradient values. However, this will cause the independent variables to iterate too slowly in the dimension with smaller gradient values. The momentum method relies on the exponentially weighted moving average (EWMA) to make the direction of the independent variable more consistent, thus reducing the possibility of divergence. In this section, we are going to introduce Adagrad [13], an algorithm that adjusts the learning rate according to the gradient value of the independent variable in each dimension to eliminate problems caused when a unified learning rate has to adapt to all dimensions.

### 12.7.1 The Algorithm

The Adagrad algorithm uses the cumulative variable  $s_t$  obtained from a square by element operation on the mini-batch stochastic gradient  $\mathbf{g}_t$ . At time step 0, Adagrad initializes each element in  $s_0$  to 0. At time step  $t$ , we first sum the results of the square by element operation for the mini-batch gradient  $\mathbf{g}_t$  to get the variable  $s_t$ :

$$\mathbf{s}_t \leftarrow \mathbf{s}_{t-1} + \mathbf{g}_t \odot \mathbf{g}_t, \quad (12.7.2)$$

Here,  $\odot$  is the symbol for multiplication by element. Next, we re-adjust the learning rate of each element in the independent variable of the objective function using element operations:

$$\mathbf{x}_t \leftarrow \mathbf{x}_{t-1} - \frac{\eta}{\sqrt{\mathbf{s}_t + \epsilon}} \odot \mathbf{g}_t, \quad (12.7.3)$$

Here,  $\eta$  is the learning rate while  $\epsilon$  is a constant added to maintain numerical stability, such as  $10^{-6}$ . Here, the square root, division, and multiplication operations are all element operations. Each element in the independent variable of the objective function will have its own learning rate after the operations by elements.

### 12.7.2 Features

We should emphasize that the cumulative variable  $s_t$  produced by a square by element operation on the mini-batch stochastic gradient is part of the learning rate denominator. Therefore, if an element in the independent variable of the objective function has a constant and large partial derivative, the learning rate of this element will drop faster. On the contrary, if the partial derivative of such an element remains small, then its learning rate will decline more slowly. However, since  $s_t$  accumulates the square by element gradient, the learning rate of each element in the independent variable declines (or remains unchanged) during iteration. Therefore, when the learning rate declines very fast during early iteration, yet the current solution is still not desirable, Adagrad might have difficulty finding a useful solution because the learning rate will be too small at later stages of iteration.

Below we will continue to use the objective function  $f(\mathbf{x}) = 0.1x_1^2 + 2x_2^2$  as an example to observe the iterative trajectory of the independent variable in Adagrad. We are going to implement Adagrad using the same learning rate as the experiment in last section, 0.4. As we can see, the iterative trajectory of the independent variable is smoother. However, due to the cumulative effect of  $s_t$ , the learning rate continuously decays, so the independent variable does not move as much during later stages of iteration.

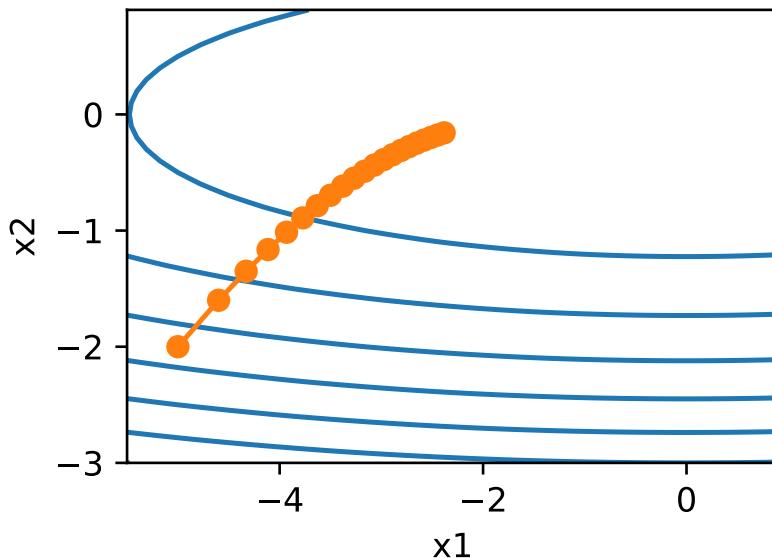
```
%matplotlib inline
import d2l
import math
from mxnet import nd

def adagrad_2d(x1, x2, s1, s2):
    # The first two terms are the independent variable gradients
    g1, g2, eps = 0.2 * x1, 4 * x2, 1e-6
    s1 += g1 ** 2
    s2 += g2 ** 2
    x1 -= eta / math.sqrt(s1 + eps) * g1
    x2 -= eta / math.sqrt(s2 + eps) * g2
    return x1, x2, s1, s2

def f_2d(x1, x2):
    return 0.1 * x1 ** 2 + 2 * x2 ** 2

eta = 0.4
d2l.show_trace_2d(f_2d, d2l.train_2d(adagrad_2d))
```

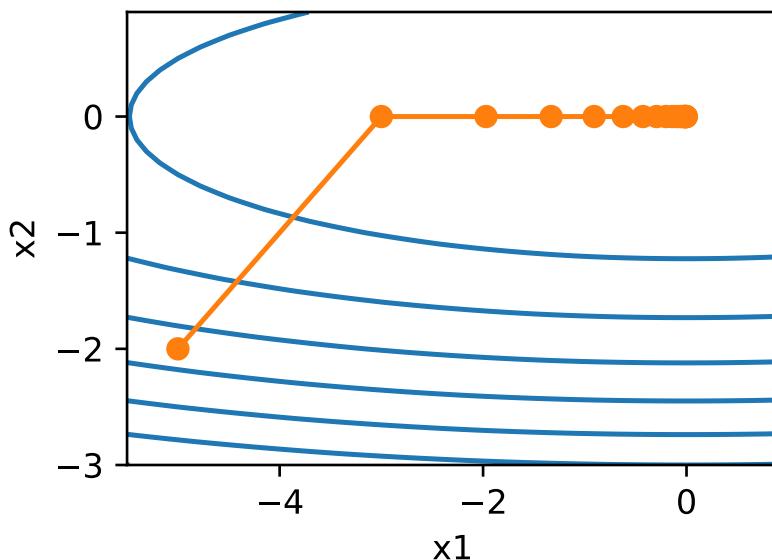
```
epoch 20, x1 -2.382563, x2 -0.158591
```



Now, we are going to increase the learning rate to 2. As we can see, the independent variable approaches the optimal solution more quickly.

```
eta = 2
d2l.show_trace_2d(f_2d, d2l.train_2d(adagrad_2d))
```

```
epoch 20, x1 -0.002295, x2 -0.000000
```



### 12.7.3 Implementation from Scratch

Like the momentum method, Adagrad needs to maintain a state variable of the same shape for each independent variable. We use the formula from the algorithm to implement Adagrad.

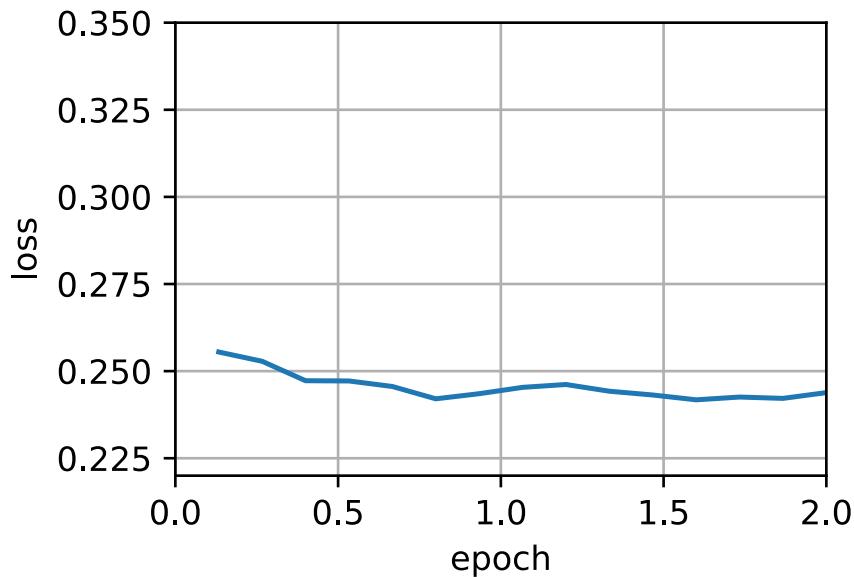
```
def init_adagrad_states(feature_dim):
    s_w = nd.zeros((feature_dim, 1))
    s_b = nd.zeros(1)
    return (s_w, s_b)

def adagrad(params, states, hyperparams):
    eps = 1e-6
    for p, s in zip(params, states):
        s[:] += p.grad.square()
        p[:] -= hyperparams['lr'] * p.grad / (s + eps).sqrt()
```

Compared with the experiment in Section 12.5, here, we use a larger learning rate to train the model.

```
data_iter, feature_dim = d2l.get_data_ch10(batch_size=10)
d2l.train_ch10(adagrad, init_adagrad_states(feature_dim),
               {'lr': 0.1}, data_iter, feature_dim);
```

```
loss: 0.244, 0.041 sec/epoch
```

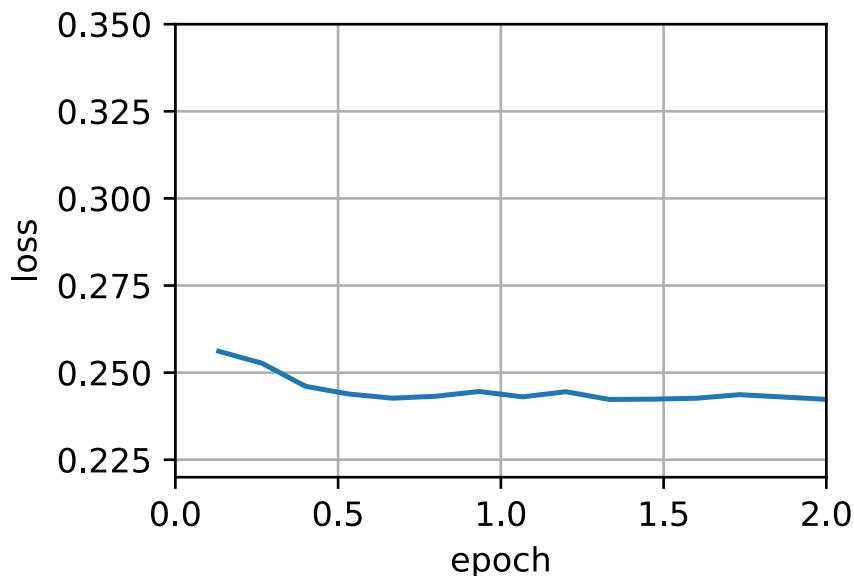


#### 12.7.4 Concise Implementation

Using the `Trainer` instance of the algorithm named “adagrad”, we can implement the Adagrad algorithm with Gluon to train models.

```
d2l.train_gluon_ch10('adagrad', {'learning_rate': 0.1}, data_iter)
```

```
loss: 0.242, 0.052 sec/epoch
```



### 12.7.5 Summary

- Adagrad constantly adjusts the learning rate during iteration to give each element in the independent variable of the objective function its own learning rate.
- When using Adagrad, the learning rate of each element in the independent variable decreases (or remains unchanged) during iteration.

### 12.7.6 Exercises

- When introducing the features of Adagrad, we mentioned a potential problem. What solutions can you think of to fix this problem?
- Try to use other initial learning rates in the experiment. How does this change the results?

### 12.7.7 Scan the QR Code to Discuss<sup>167</sup>



## 12.8 RMSProp

In the experiment in Section 12.7, the learning rate of each element in the independent variable of the objective function declines (or remains unchanged) during iteration because the variable  $\mathbf{s}_t$  in the denominator is increased by the square by element operation of the mini-batch stochastic gradient, adjusting the learning rate. Therefore, when the learning rate declines very fast during early iteration, yet the current solution is still not desirable, Adagrad might have difficulty finding a useful solution because the learning rate will be too small at later stages of iteration. To tackle this problem, the RMSProp algorithm [61] made a small modification to Adagrad.

### 12.8.1 The Algorithm

Unlike in Adagrad, the state variable  $\mathbf{s}_t$  is the sum of the square by element all the mini-batch stochastic gradients  $\mathbf{g}_t$  up to the time step  $t$ , RMSProp uses the exponentially weighted moving average on the square by element results of these gradients. Specifically, given the hyperparameter  $0 \leq \gamma < 1$ , RMSProp is computed at time step  $t > 0$ .

$$\mathbf{s}_t \leftarrow \gamma \mathbf{s}_{t-1} + (1 - \gamma) \mathbf{g}_t \odot \mathbf{g}_t. \quad (12.8.1)$$

Like Adagrad, RMSProp re-adjusts the learning rate of each element in the independent variable of the objective function with element operations and then updates the independent variable.

$$\mathbf{x}_t \leftarrow \mathbf{x}_{t-1} - \frac{\eta}{\sqrt{\mathbf{s}_t + \epsilon}} \odot \mathbf{g}_t, \quad (12.8.2)$$

Here,  $\eta$  is the learning rate while  $\epsilon$  is a constant added to maintain numerical stability, such as  $10^{-6}$ .

<sup>167</sup> <https://discuss.mxnet.io/t/2375>

### Exponentially Weighted Moving Average (EWMA)

Now let expand the definition of  $\mathbf{s}_t$ , we can see that

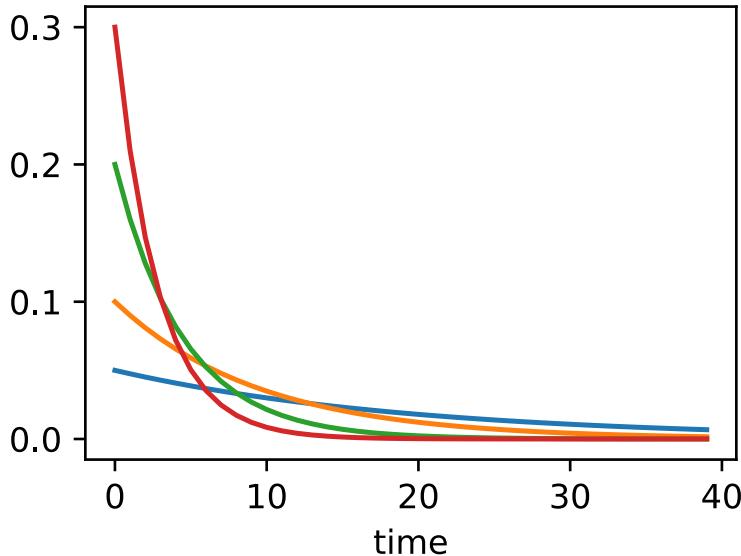
$$\begin{aligned}\mathbf{s}_t &= (1 - \gamma)\mathbf{g}_t \odot \mathbf{g}_t + \gamma\mathbf{s}_{t-1} \\ &= (1 - \gamma)(\mathbf{g}_t \odot \mathbf{g}_t + \gamma\mathbf{g}_{t-1} \odot \mathbf{g}_{t-1}) + \gamma^2\mathbf{s}_{t-2} \\ &\dots \\ &= (1 - \gamma)(\mathbf{g}_t \odot \mathbf{g}_t + \gamma\mathbf{g}_{t-1} \odot \mathbf{g}_{t-1} + \dots + \gamma^{t-1}\mathbf{g}_1 \odot \mathbf{g}_1).\end{aligned}\tag{12.8.3}$$

In Section 12.6 we see that  $\frac{1}{1-\gamma} = 1 + \gamma + \gamma^2 + \dots$ , so the sum of weights equals to 1. In addition, these weights decrease exponentially, it is called exponentially weighted moving average.

We visualize the weights in the past 40 time steps with various  $\gamma$ s.

```
%matplotlib inline
import d2l
import math
from mxnet import nd

gammas = [0.95, 0.9, 0.8, 0.7]
d2l.set_figsize((3.5, 2.5))
for gamma in gammas:
    x = nd.arange(40).asnumpy()
    d2l.plt.plot(x, (1-gamma) * gamma ** x, label='gamma = %.2f'%gamma)
d2l.plt.xlabel('time');
```



### 12.8.2 Implementation from Scratch

By convention, we will use the objective function  $f(\mathbf{x}) = 0.1x_1^2 + 2x_2^2$  to observe the iterative trajectory of the independent variable in RMSProp. Recall that in Section 12.7, when we used Adagrad with a learning rate of 0.4, the independent variable moved less in later stages of iteration. However, at the same learning rate, RMSProp can approach the optimal solution faster.

```

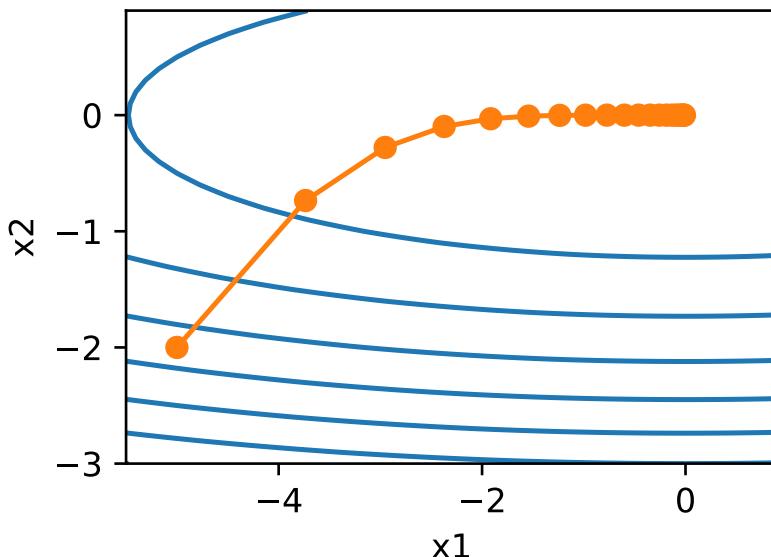
def rmsprop_2d(x1, x2, s1, s2):
    g1, g2, eps = 0.2 * x1, 4 * x2, 1e-6
    s1 = gamma * s1 + (1 - gamma) * g1 ** 2
    s2 = gamma * s2 + (1 - gamma) * g2 ** 2
    x1 -= eta / math.sqrt(s1 + eps) * g1
    x2 -= eta / math.sqrt(s2 + eps) * g2
    return x1, x2, s1, s2

def f_2d(x1, x2):
    return 0.1 * x1 ** 2 + 2 * x2 ** 2

eta, gamma = 0.4, 0.9
d2l.show_trace_2d(f_2d, d2l.train_2d(rmsprop_2d))

```

epoch 20, x1 -0.010599, x2 0.000000



Next, we implement RMSProp with the formula in the algorithm.

```

def init_rmsprop_states(feature_dim):
    s_w = nd.zeros((feature_dim, 1))
    s_b = nd.zeros(1)
    return (s_w, s_b)

def rmsprop(params, states, hyperparams):
    gamma, eps = hyperparams['gamma'], 1e-6
    for p, s in zip(params, states):
        s[:] = gamma * s + (1 - gamma) * p.grad.square()
        p[:] -= hyperparams['lr'] * p.grad / (s + eps).sqrt()

```

We set the initial learning rate to 0.01 and the hyperparameter  $\gamma$  to 0.9. Now, the variable  $s_t$  can be treated as the weighted average of the square term  $\mathbf{g}_t \odot \mathbf{g}_t$  from the last  $1/(1 - 0.9) = 10$  time steps.

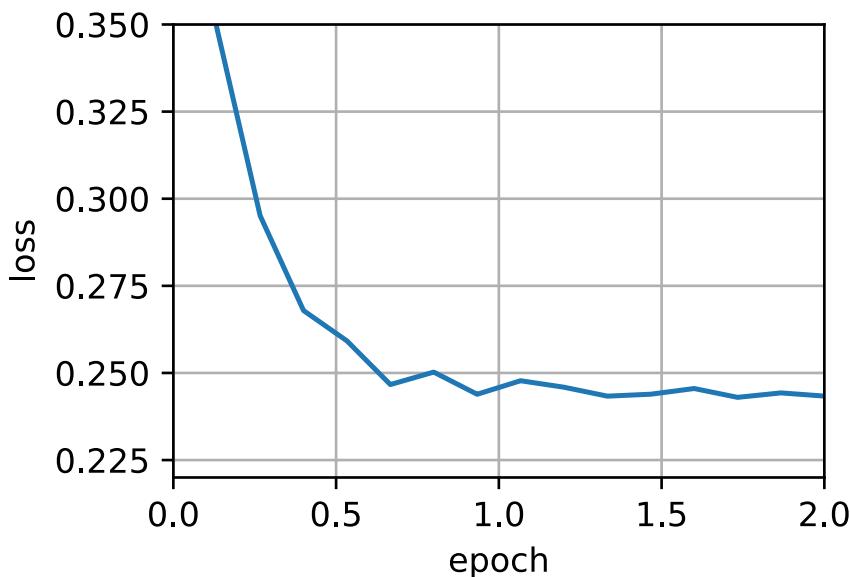
data\_iter, feature\_dim = d2l.get\_data\_ch10(batch\_size=10)

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```
d2l.train_ch10(rmsprop, init_rmsprop_states(feature_dim),  
{'lr': 0.01, 'gamma': 0.9}, data_iter, feature_dim);
```

```
loss: 0.243, 0.042 sec/epoch
```

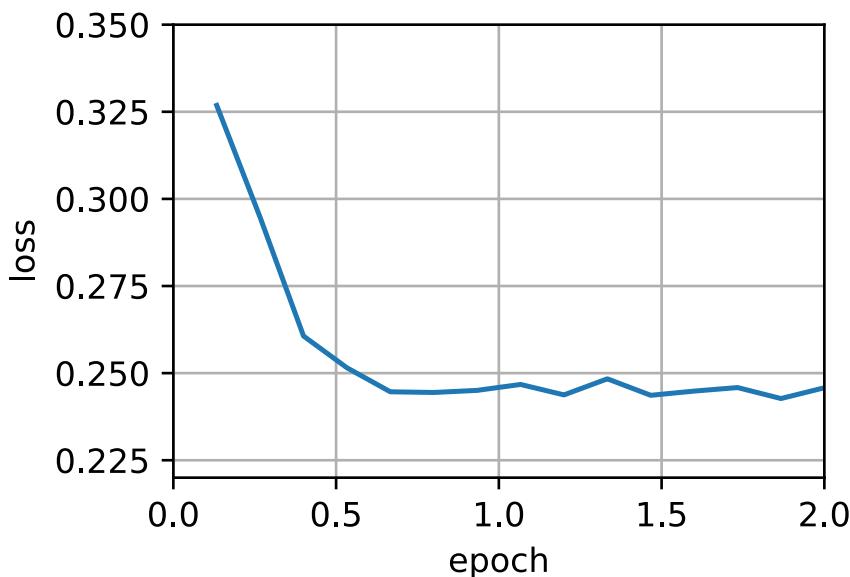


### 12.8.3 Concise Implementation

From the `Trainer` instance of the algorithm named “rmsprop”, we can implement the RMSProp algorithm with Gluon to train models. Note that the hyperparameter  $\gamma$  is assigned by `gamma1`.

```
d2l.train_gluon_ch10('rmsprop', {'learning_rate': 0.01, 'gamma1': 0.9},  
data_iter)
```

```
loss: 0.246, 0.025 sec/epoch
```



#### 12.8.4 Summary

- The difference between RMSProp and Adagrad is that RMSProp uses an EWMA on the squares of elements in the mini-batch stochastic gradient to adjust the learning rate.

#### 12.8.5 Exercises

- What happens to the experimental results if we set the value of  $\gamma$  to 1? Why?
- Try using other combinations of initial learning rates and  $\gamma$  hyperparameters and observe and analyze the experimental results.

#### 12.8.6 Scan the QR Code to Discuss<sup>168</sup>



### 12.9 Adadelta

In addition to RMSProp, Adadelta is another common optimization algorithm that helps improve the chances of finding useful solutions at later stages of iteration, which is difficult to do when using the Adagrad algorithm for the same purpose [70]. The interesting thing is that there is no learning rate hyperparameter in the Adadelta algorithm.

<sup>168</sup> <https://discuss.mxnet.io/t/2376>

### 12.9.1 The Algorithm

Like RMSProp, the Adadelta algorithm uses the variable  $s_t$ , which is an EWMA on the squares of elements in mini-batch stochastic gradient  $\mathbf{g}_t$ . At time step 0, all the elements are initialized to 0. Given the hyperparameter  $0 \leq \rho < 1$  (counterpart of  $\gamma$  in RMSProp), at time step  $t > 0$ , compute using the same method as RMSProp:

$$\mathbf{s}_t \leftarrow \rho \mathbf{s}_{t-1} + (1 - \rho) \mathbf{g}_t \odot \mathbf{g}_t. \quad (12.9.1)$$

Unlike RMSProp, Adadelta maintains an additional state variable,  $\Delta\mathbf{x}_t$  the elements of which are also initialized to 0 at time step 0. We use  $\Delta\mathbf{x}_{t-1}$  to compute the variation of the independent variable:

$$\mathbf{g}'_t \leftarrow \sqrt{\frac{\Delta\mathbf{x}_{t-1} + \epsilon}{s_t + \epsilon}} \odot \mathbf{g}_t, \quad (12.9.2)$$

Here,  $\epsilon$  is a constant added to maintain the numerical stability, such as  $10^{-5}$ . Next, we update the independent variable:

$$\mathbf{x}_t \leftarrow \mathbf{x}_{t-1} - \mathbf{g}'_t. \quad (12.9.3)$$

Finally, we use  $\Delta\mathbf{x}$  to record the EWMA on the squares of elements in  $\mathbf{g}'$ , which is the variation of the independent variable.

$$\Delta\mathbf{x}_t \leftarrow \rho \Delta\mathbf{x}_{t-1} + (1 - \rho) \mathbf{g}'_t \odot \mathbf{g}'_t. \quad (12.9.4)$$

As we can see, if the impact of  $\epsilon$  is not considered here, Adadelta differs from RMSProp in its replacement of the hyperparameter  $\eta$  with  $\sqrt{\Delta\mathbf{x}_{t-1}}$ .

### 12.9.2 Implementation from Scratch

Adadelta needs to maintain two state variables for each independent variable,  $s_t$  and  $\Delta\mathbf{x}_t$ . We use the formula from the algorithm to implement Adadelta.

```
%matplotlib inline
import d2l
from mxnet import nd

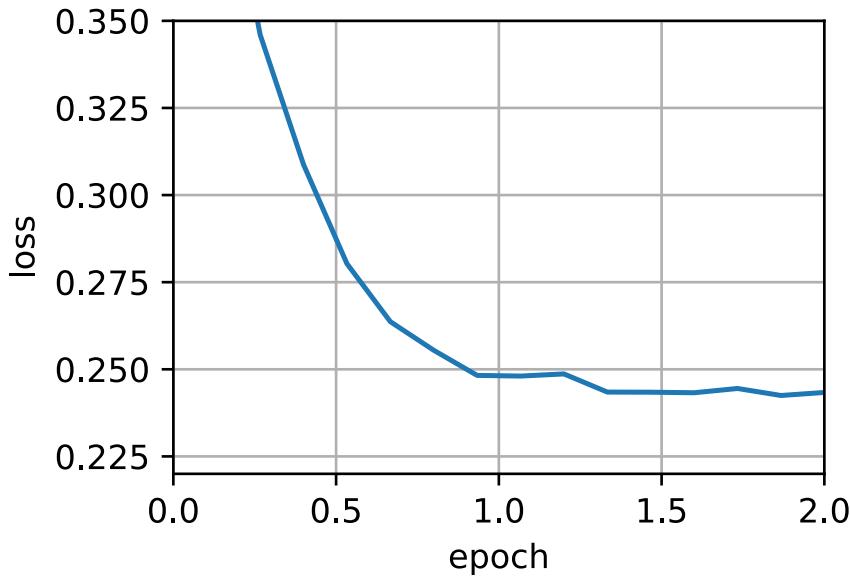
def init_adadelta_states(feature_dim):
    s_w, s_b = nd.zeros((feature_dim, 1)), nd.zeros(1)
    delta_w, delta_b = nd.zeros((feature_dim, 1)), nd.zeros(1)
    return ((s_w, delta_w), (s_b, delta_b))

def adadelta(params, states, hyperparams):
    rho, eps = hyperparams['rho'], 1e-5
    for p, (s, delta) in zip(params, states):
        s[:] = rho * s + (1 - rho) * p.grad.square()
        g = ((delta + eps).sqrt() / (s + eps).sqrt()) * p.grad
        p[:] -= g
        delta[:] = rho * delta + (1 - rho) * g * g
```

Then, we train the model with the hyperparameter  $\rho = 0.9$ .

```
data_iter, feature_dim = d2l.get_data_ch10(batch_size=10)
d2l.train_ch10(adadelta, init_adadelta_states(feature_dim),
    {'rho': 0.9}, data_iter, feature_dim);
```

```
loss: 0.243, 0.049 sec/epoch
```

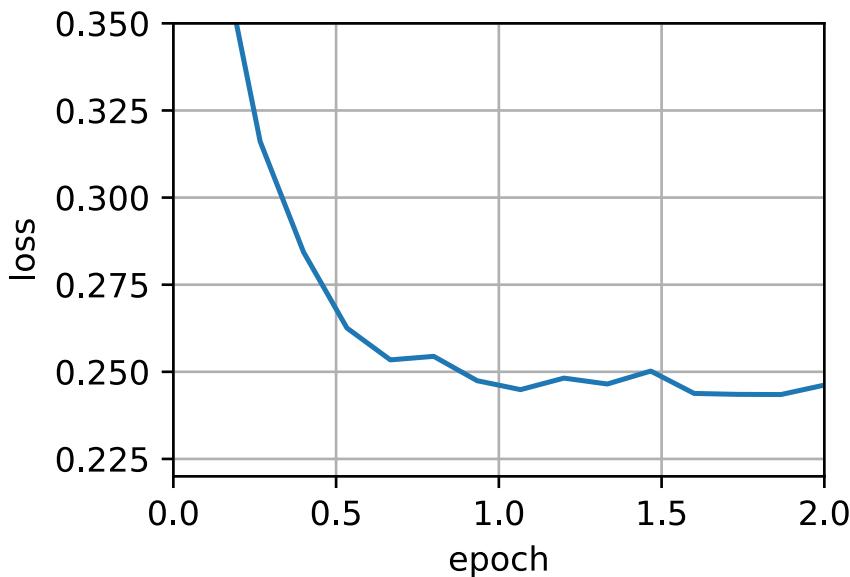


### 12.9.3 Concise Implementation

From the `Trainer` instance for the algorithm named “`adadelta`”, we can implement Adadelta in Gluon. Its hyperparameters can be specified by `rho`.

```
d2l.train_gluon_ch10('adadelta', {'rho': 0.9}, data_iter)
```

```
loss: 0.246, 0.056 sec/epoch
```



### 12.9.4 Summary

- Adadelta has no learning rate hyperparameter, it uses an EWMA on the squares of elements in the variation of the independent variable to replace the learning rate.

### 12.9.5 Exercises

- Adjust the value of  $\rho$  and observe the experimental results.

### 12.9.6 Scan the QR Code to Discuss<sup>169</sup>



## 12.10 Adam

Created on the basis of RMSProp, Adam also uses EWMA on the mini-batch stochastic gradient[1]. Here, we are going to introduce this algorithm.

### 12.10.1 The Algorithm

Adam [31] uses the momentum variable  $\mathbf{v}_t$  and variable  $\mathbf{s}_t$ , which is an EWMA on the squares of elements in the mini-batch stochastic gradient from RMSProp, and initializes each element of the variables to 0 at time step 0. Given the hyperparameter  $0 \leq \beta_1 < 1$  (the author of the algorithm suggests a value of 0.9), the momentum variable  $\mathbf{v}_t$  at time step  $t$  is the EWMA of the mini-batch stochastic gradient  $\mathbf{g}_t$ :

$$\mathbf{v}_t \leftarrow \beta_1 \mathbf{v}_{t-1} + (1 - \beta_1) \mathbf{g}_t. \quad (12.10.1)$$

Just as in RMSProp, given the hyperparameter  $0 \leq \beta_2 < 1$  (the author of the algorithm suggests a value of 0.999), After taken the squares of elements in the mini-batch stochastic gradient, find  $\mathbf{g}_t \odot \mathbf{g}_t$  and perform EWMA on it to obtain  $\mathbf{s}_t$ :

$$\mathbf{s}_t \leftarrow \beta_2 \mathbf{s}_{t-1} + (1 - \beta_2) \mathbf{g}_t \odot \mathbf{g}_t. \quad (12.10.2)$$

Since we initialized elements in  $\mathbf{v}_0$  and  $\mathbf{s}_0$  to 0, we get  $\mathbf{v}_t = (1 - \beta_1) \sum_{i=1}^t \beta_1^{t-i} \mathbf{g}_i$  at time step  $t$ . Sum the mini-batch stochastic gradient weights from each previous time step to get  $(1 - \beta_1) \sum_{i=1}^t \beta_1^{t-i} = 1 - \beta_1^t$ . Notice that when  $t$  is small, the sum of the mini-batch stochastic gradient weights from each previous time step will be small. For example, when  $\beta_1 = 0.9$ ,  $\mathbf{v}_1 = 0.1\mathbf{g}_1$ . To eliminate this effect, for any time step  $t$ , we can divide  $\mathbf{v}_t$  by  $1 - \beta_1^t$ , so that the sum of the mini-batch stochastic gradient weights from each previous time step is 1. This is also called bias correction. In the Adam algorithm, we perform bias corrections for variables  $\mathbf{v}_t$  and  $\mathbf{s}_t$ :

$$\hat{\mathbf{v}}_t \leftarrow \frac{\mathbf{v}_t}{1 - \beta_1^t}, \quad (12.10.3)$$

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<sup>169</sup> <https://discuss.mxnet.io/t/2377>

$$\hat{s}_t \leftarrow \frac{s_t}{1 - \beta_2^t}. \quad (12.10.4)$$

Next, the Adam algorithm will use the bias-corrected variables  $\hat{v}_t$  and  $\hat{s}_t$  from above to re-adjust the learning rate of each element in the model parameters using element operations.

$$\mathbf{g}'_t \leftarrow \frac{\eta \hat{v}_t}{\sqrt{\hat{s}_t} + \epsilon}, \quad (12.10.5)$$

Here,  $\eta$  is the learning rate while  $\epsilon$  is a constant added to maintain numerical stability, such as  $10^{-8}$ . Just as for Adagrad, RMSProp, and Adadelta, each element in the independent variable of the objective function has its own learning rate. Finally, use  $\mathbf{g}'_t$  to iterate the independent variable:

$$\mathbf{x}_t \leftarrow \mathbf{x}_{t-1} - \mathbf{g}'_t. \quad (12.10.6)$$

### 12.10.2 Implementation from Scratch

We use the formula from the algorithm to implement Adam. Here, time step  $t$  uses `hyperparams` to input parameters to the `adam` function.

```
%matplotlib inline
import d2l
from mxnet import nd

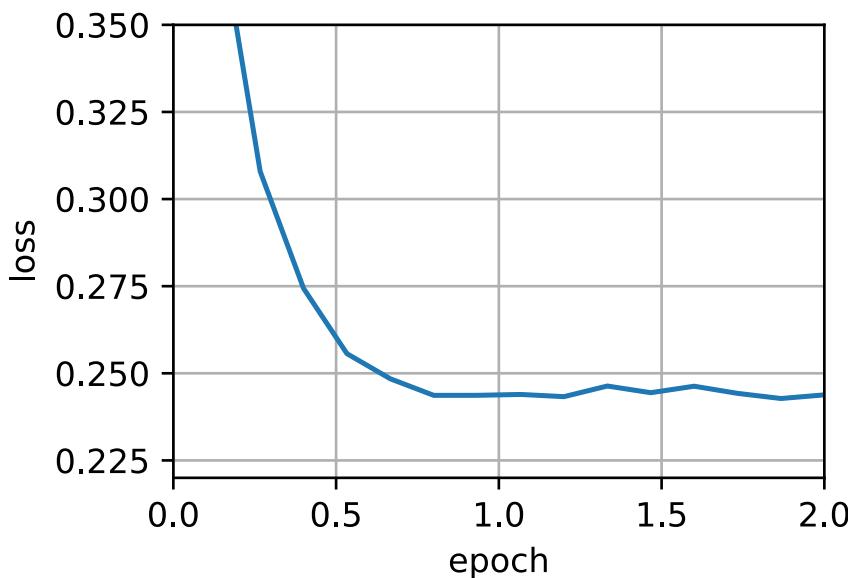
def init_adam_states(feature_dim):
    v_w, v_b = nd.zeros((feature_dim, 1)), nd.zeros(1)
    s_w, s_b = nd.zeros((feature_dim, 1)), nd.zeros(1)
    return ((v_w, s_w), (v_b, s_b))

def adam(params, states, hyperparams):
    beta1, beta2, eps = 0.9, 0.999, 1e-6
    for p, (v, s) in zip(params, states):
        v[:] = beta1 * v + (1 - beta1) * p.grad
        s[:] = beta2 * s + (1 - beta2) * p.grad.square()
        v_bias_corr = v / (1 - beta1 ** hyperparams['t'])
        s_bias_corr = s / (1 - beta2 ** hyperparams['t'])
        p[:] -= hyperparams['lr'] * v_bias_corr / (s_bias_corr.sqrt() + eps)
    hyperparams['t'] += 1
```

Use Adam to train the model with a learning rate of 0.01.

```
data_iter, feature_dim = d2l.get_data_ch10(batch_size=10)
d2l.train_ch10(adam, init_adam_states(feature_dim),
               {'lr': 0.01, 't': 1}, data_iter, feature_dim);
```

```
loss: 0.244, 0.051 sec/epoch
```

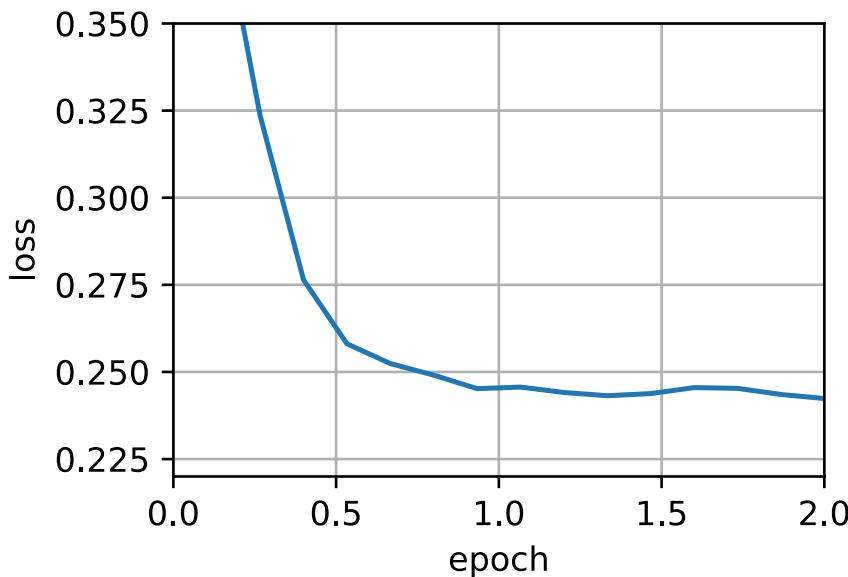


### 12.10.3 Concise Implementation

From the Trainer instance of the algorithm named “adam”, we can implement Adam with Gluon.

```
d2l.train_gluon_ch10('adam', {'learning_rate': 0.01}, data_iter)
```

```
loss: 0.242, 0.030 sec/epoch
```



#### 12.10.4 Summary

- Created on the basis of RMSProp, Adam also uses EWMA on the mini-batch stochastic gradient
- Adam uses bias correction.

#### 12.10.5 Exercises

- Adjust the learning rate and observe and analyze the experimental results.
- Some people say that Adam is a combination of RMSProp and momentum. Why do you think they say this?

#### 12.10.6 Scan the QR Code to Discuss<sup>170</sup>



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<sup>170</sup> <https://discuss.mxnet.io/t/2378>



## COMPUTATIONAL PERFORMANCE

In deep learning, data sets are usually large and model computation is complex. Therefore, we are always very concerned about computing performance. This chapter will focus on the important factors that affect computing performance: imperative programming, symbolic programming, asynchronous programming, automatic parallel computation, and multi-GPU computation. By studying this chapter, you should be able to further improve the computing performance of the models that have been implemented in the previous chapters, for example, by reducing the model training time without affecting the accuracy of the model.

### 13.1 A Hybrid of Imperative and Symbolic Programming

So far, this book has focused on imperative programming, which makes use of programming statements to change a program's state. Consider the following example of simple imperative programming code.

```
def add(a, b):
    return a + b

def fancy_func(a, b, c, d):
    e = add(a, b)
    f = add(c, d)
    g = add(e, f)
    return g

fancy_func(1, 2, 3, 4)
```

10

As expected, Python will perform an addition when running the statement `e = add(a, b)`, and will store the result as the variable `e`, thereby changing the program's state. The next two statements `f = add(c, d)` and `g = add(e, f)` will similarly perform additions and store the results as variables.

Although imperative programming is convenient, it may be inefficient. On the one hand, even if the `add` function is repeatedly called throughout the `fancy_func` function, Python will execute the three function calling statements individually, one after the other. On the other hand, we need to save the variable values of `e` and `f` until all the statements in `fancy_func` have been executed. This is because we do not know whether the variables `e` and `f` will be used by other parts of the program after the statements `e = add(a, b)` and `f = add(c, d)` have been executed.

Contrary to imperative programming, symbolic programming is usually performed after the computational process has been fully defined. Symbolic programming is used by multiple deep learning frameworks, including Theano and TensorFlow. The process of symbolic programming generally requires the following three steps:

1. Define the computation process.
2. Compile the computation process into an executable program.
3. Provide the required inputs and call on the compiled program for execution.

In the example below, we utilize symbolic programming to re-implement the imperative programming code provided at the beginning of this section.

```
def add_str():
    return ''
def add(a, b):
    return a + b
...

def fancy_func_str():
    return ''
def fancy_func(a, b, c, d):
    e = add(a, b)
    f = add(c, d)
    g = add(e, f)
    return g
...

def evoke_str():
    return add_str() + fancy_func_str() + ''
print(fancy_func(1, 2, 3, 4))
...

prog = evoke_str()
print(prog)
y = compile(prog, '', 'exec')
exec(y)
```

```
def add(a, b):
    return a + b

def fancy_func(a, b, c, d):
    e = add(a, b)
    f = add(c, d)
    g = add(e, f)
    return g

print(fancy_func(1, 2, 3, 4))
```

10

The three functions defined above will only return the results of the computation process as a string. Finally, the complete computation process is compiled and run using the `compile` function. This leaves more room to optimize computation, since the system is able to view the entire program during its compilation. For example, during compilation, the program can be rewritten as `print((1 + 2) + (3 + 4))` or even directly rewritten as `print(10)`. Apart from reducing the amount of function calls, this process also saves memory.

A comparison of these two programming methods shows that

- imperative programming is easier. When imperative programming is used in Python, the majority

of the code is straightforward and easy to write. At the same time, it is easier to debug imperative programming code. This is because it is easier to obtain and print all relevant intermediate variable values, or make use of Python's built-in debugging tools.

- Symbolic programming is more efficient and easier to port. Symbolic programming makes it easier to better optimize the system during compilation, while also having the ability to port the program into a format independent of Python. This allows the program to be run in a non-Python environment, thus avoiding any potential performance issues related to the Python interpreter.

### 13.1.1 Hybrid programming provides the best of both worlds.

Most deep learning frameworks choose either imperative or symbolic programming. For example, both Theano and TensorFlow (inspired by the latter) make use of symbolic programming, while Chainer and PyTorch utilize imperative programming. When designing Gluon, developers considered whether it was possible to harness the benefits of both imperative and symbolic programming. The developers believed that users should be able to develop and debug using pure imperative programming, while having the ability to convert most programs into symbolic programming to be run when product-level computing performance and deployment are required. This was achieved by Gluon through the introduction of hybrid programming.

In hybrid programming, we can build models using either the `HybridBlock` or the `HybridSequential` classes. By default, they are executed in the same way `Block` or `Sequential` classes are executed in imperative programming. When the `hybridize` function is called, Gluon will convert the program's execution into the style used in symbolic programming. In fact, most models can make use of hybrid programming's execution style.

Through the use of experiments, this section will demonstrate the benefits of hybrid programming.

### 13.1.2 Constructing Models Using the `HybridSequential` Class

Previously, we learned how to use the `Sequential` class to concatenate multiple layers. Next, we will replace the `Sequential` class with the `HybridSequential` class in order to make use of hybrid programming.

```
from mxnet import nd, sym
from mxnet.gluon import nn
import time

def get_net():
    net = nn.HybridSequential() # Here we use the class HybridSequential
    net.add(nn.Dense(256, activation='relu'),
            nn.Dense(128, activation='relu'),
            nn.Dense(2))
    net.initialize()
    return net

x = nd.random.normal(shape=(1, 512))
net = get_net()
net(x)
```

```
[[0.08827581 0.00505182]]
<NDArray 1x2 @cpu(0)>
```

By calling the `hybridize` function, we are able to compile and optimize the computation of the concatenation layer in the `HybridSequential` instance. The model's computation result remains unchanged.

```
net.hybridize()  
net(x)
```

```
[[0.08827581 0.00505182]]  
<NDArray 1x2 @cpu(0)>
```

It should be noted that only the layers inheriting the `HybridBlock` class will be optimized during computation. For example, the `HybridSequential` and `Dense` classes provided by Gluon are all subclasses of `HybridBlock` class, meaning they will both be optimized during computation. A layer will not be optimized if it inherits from the `Block` class rather than the `HybridBlock` class.

## Computing Performance

To demonstrate the performance improvement gained by the use of symbolic programming, we will compare the computation time before and after calling the `hybridize` function. Here we time 1000 `net` model computations. The model computations are based on imperative and symbolic programming, respectively, before and after `net` has called the `hybridize` function.

```
def benchmark(net, x):  
    start = time.time()  
    for i in range(1000):  
        _ = net(x)  
    # To facilitate timing, we wait for all computations to be completed  
    nd.waitall()  
    return time.time() - start  
  
net = get_net()  
print('before hybridizing: %.4f sec' % (benchmark(net, x)))  
net.hybridize()  
print('after hybridizing: %.4f sec' % (benchmark(net, x)))
```

```
before hybridizing: 0.3183 sec  
after hybridizing: 0.2622 sec
```

As is observed in the above results, after a `HybridSequential` instance calls the `hybridize` function, computing performance is improved through the use of symbolic programming.

## Achieving Symbolic Programming

We can save the symbolic program and model parameters to the hard disk through the use of the `export` function after the `net` model has finished computing the output based on the input, such as in the case of `net(x)` in the `benchmark` function.

```
net.export('my_mlp')
```

The `.json` and `.params` files generated during this process are a symbolic program and a model parameter, respectively. They can be read by other front-end languages supported by Python or MXNet, such as C++, R, Scala, and Perl. This allows us to deploy trained models to other devices and easily use other front-end programming languages. At the same time, because symbolic programming was used during deployment, the computing performance is often superior to that based on imperative programming.

In MXNet, a symbolic program refers to a program that makes use of the `Symbol` type. We know that, when the `NDArray` input `x` is provided to `net`, `net(x)` will directly calculate the model output and return a result

based on `x`. For models that have called the `hybridize` function, we can also provide a Symbol-type input variable, and `net(x)` will return Symbol type results.

```
x = sym.var('data')
net(x)
```

```
<Symbol dense5_fwd>
```

### 13.1.3 Constructing Models Using the HybridBlock Class

Similar to the correlation between the Sequential Block classes, the `HybridSequential` class is a `HybridBlock` subclass. Contrary to the Block instance, which needs to use the `forward` function, for a `HybridBlock` instance we need to use the `hybrid_forward` function.

Earlier, we demonstrated that, after calling the `hybridize` function, the model is able to achieve superior computing performance and portability. In addition, model flexibility can be affected after calling the `hybridize` function. We will demonstrate this by constructing a model using the `HybridBlock` class.

```
class HybridNet(nn.HybridBlock):
    def __init__(self, **kwargs):
        super(HybridNet, self).__init__(**kwargs)
        self.hidden = nn.Dense(10)
        self.output = nn.Dense(2)

    def hybrid_forward(self, F, x):
        print('F: ', F)
        print('x: ', x)
        x = F.relu(self.hidden(x))
        print('hidden: ', x)
        return self.output(x)
```

We need to add the additional input `F` to the `hybrid_forward` function when inheriting the `HybridBlock` class. We already know that MXNet uses both an `NDArray` class and a `Symbol` class, which are based on imperative programming and symbolic programming, respectively. Since these two classes perform very similar functions, MXNet will determine whether `F` will call `NDArray` or `Symbol` based on the input provided.

The following creates a `HybridBlock` instance. As we can see, by default, `F` uses `NDArray`. We also printed out the `x` input as well as the hidden layer's output using the ReLU activation function.

```
net = HybridNet()
net.initialize()
x = nd.random.normal(shape=(1, 4))
net(x)
```

```
F: <module 'mxnet.ndarray' from '/var/lib/jenkins/miniconda3/envs/d2l-en-build-0/lib/
˓→python3.7/site-packages/mxnet/ndarray/__init__.py'>
x:
[[ -0.12225834  0.5429998 -0.9469352   0.59643304 ]]
<NDArray 1x4 @cpu(0)>
hidden:
[[ 0.11134676  0.04770704  0.05341475  0.          0.08091211  0.
  0.          0.04143535  0.          0.          ]]
<NDArray 1x10 @cpu(0)>
```

```
[[0.00370749 0.00134991]]  
<NDArray 1x2 @cpu(0)>
```

Repeating the forward computation will achieve the same results.

```
net(x)
```

```
F: <module 'mxnet.ndarray' from '/var/lib/jenkins/miniconda3/envs/d2l-en-build-0/lib/  
˓→python3.7/site-packages/mxnet/ndarray/__init__.py'>  
x:  
[[[-0.12225834 0.5429998 -0.9469352 0.59643304]]]  
<NDArray 1x4 @cpu(0)>  
hidden:  
[[[0.11134676 0.04770704 0.05341475 0. 0.08091211 0.  
0. 0.04143535 0. 0. ]]  
<NDArray 1x10 @cpu(0)>
```

```
[[0.00370749 0.00134991]]  
<NDArray 1x2 @cpu(0)>
```

Next, we will see what happens after we call the `hybridize` function.

```
net.hybridize()  
net(x)
```

```
F: <module 'mxnet.symbol' from '/var/lib/jenkins/miniconda3/envs/d2l-en-build-0/lib/  
˓→python3.7/site-packages/mxnet/symbol/__init__.py'>  
x: <Symbol data>  
hidden: <Symbol hybridnet0_relu0>
```

```
[[0.00370749 0.00134991]]  
<NDArray 1x2 @cpu(0)>
```

We can see that `F` turns into a `Symbol`. Moreover, even though the input data is still `NDArray`, the same input and intermediate output will all be converted to `Symbol` type in the `hybrid_forward` function.

Now, we repeat the forward computation.

```
net(x)
```

```
[[0.00370749 0.00134991]]  
<NDArray 1x2 @cpu(0)>
```

We can see that the three lines of print statements defined in the `hybrid_forward` function will not print anything. This is because a symbolic program has been produced since the last time `net(x)` was run by calling the `hybridize` function. Afterwards, when we run `net(x)` again, MXNet will no longer need to access Python code, but can directly perform symbolic programming at the C++ backend. This is another reason why model computing performance will be improve after the `hybridize` function is called. However, there is always the potential that any programs we write will suffer a loss in flexibility. If we want to use the three lines of print statements to debug the code in the above example, they will be skipped over and we would not be able to print when the symbolic program is executed. Additionally, in the case of a few functions not supported by `Symbol` (like `asnumpy`), and operations in-place like `a += b` and `a[:] = a + b`

(must be rewritten as `a = a + b`). Therefore, we will not be able to use the `hybrid_forward` function or perform forward computation after the `hybridize` function has been called.

### 13.1.4 Summary

- Both imperative and symbolic programming have their advantages as well as their disadvantages. Through hybrid programming, MXNet is able to combine the advantages of both.
- Models constructed by the `HybridSequential` and `HybridBlock` classes are able to convert imperative program into symbolic program by calling the `hybridize` function. We recommend using this method to improve computing performance.

### 13.1.5 Exercises

- Add `x.asnumpy()` to the first line of the `hybrid_forward` function of the `HybridNet` class in this section, run all the code in this section, and observe any error types and locations
- What happens if we add the Python statements `if` and `for` in the `hybrid_forward` function?
- Review the models that interest you in the previous chapters and use the `HybridBlock` class or `HybridSequential` class to implement them.

### 13.1.6 Scan the QR Code to Discuss<sup>171</sup>



## 13.2 Asynchronous Computing

MXNet utilizes asynchronous programming to improve computing performance. Understanding how asynchronous programming works helps us to develop more efficient programs, by proactively reducing computational requirements and thereby minimizing the memory overhead required in the case of limited memory resources. First, we will import the package or module needed for this section's experiment.

```
import d2l
from mxnet import autograd, gluon, nd
from mxnet.gluon import nn
import os
import subprocess
```

### 13.2.1 Asynchronous Programming in MXNet

Broadly speaking, MXNet includes the front-end directly used by users for interaction, as well as the back-end used by the system to perform the computation. For example, users can write MXNet programs in

<sup>171</sup> <https://discuss.mxnet.io/t/2380>

various front-end languages, such as Python, R, Scala and C++. Regardless of the front-end programming language used, the execution of MXNet programs occurs primarily in the back-end of C++ implementations. In other words, front-end MXNet programs written by users are passed on to the back-end to be computed. The back-end possesses its own threads that continuously collect and execute queued tasks.

Through the interaction between front-end and back-end threads, MXNet is able to implement asynchronous programming. Asynchronous programming means that the front-end threads continue to execute subsequent instructions without having to wait for the back-end threads to return the results from the current instruction. For simplicity's sake, assume that the Python front-end thread calls the following four instructions.

```
a = nd.ones((1, 2))
b = nd.ones((1, 2))
c = a * b + 2
c
```

```
[[3. 3.]]
<NDArray 1x2 @cpu(0)>
```

In Asynchronous Computing, whenever the Python front-end thread executes one of the first three statements, it simply returns the task to the back-end queue. When the last statement's results need to be printed, the Python front-end thread will wait for the C++ back-end thread to finish computing result of the variable `c`. One benefit of such as design is that the Python front-end thread in this example does not need to perform actual computations. Thus, there is little impact on the program's overall performance, regardless of Python's performance. MXNet will deliver consistently high performance, regardless of the front-end language's performance, provided the C++ back-end can meet the efficiency requirements.

The following example uses timing to demonstrate the effect of asynchronous programming. As we can see, when `y = nd.dot(x, x).sum()` is returned, it does not actually wait for the variable `y` to be calculated. Only when the `print` function needs to print the variable `y` must the function wait for it to be calculated.

```
timer = d2l.Timer()
x = nd.random.uniform(shape=(2000, 2000))
y = nd.dot(x, x).sum()
print('Workloads are queued. Time %.4f sec' % timer.stop())

print('sum =', y)
print('Workloads are finished. Time %.4f sec' % timer.stop())
```

```
Workloads are queued. Time 0.0009 sec
sum =
[2.0003661e+09]
<NDArray 1 @cpu(0)>
Workloads are finished. Time 0.1519 sec
```

In truth, whether or not the current result is already calculated in the memory is irrelevant, unless we need to print or save the computation results. So long as the data is stored in NDArray and the operators provided by MXNet are used, MXNet will utilize asynchronous programming by default to attain superior computing performance.

### 13.2.2 Use of the Synchronization Function to Allow the Front-End to Wait for the Computation Results

In addition to the `print` function we just introduced, there are other ways to make the front-end thread wait for the completion of the back-end computations. The `wait_to_read` function can be used to make the

front-end wait for the complete computation of the NDArray results, and then execute following statement. Alternatively, we can use the `waitall` function to make the front-end wait for the completion of all previous computations. The latter is a common method used in performance testing.

Below, we use the `wait_to_read` function as an example. The time output includes the calculation time of `y`.

```
timer.start()
y = nd.dot(x, x)
y.wait_to_read()
print('Done in %.4f sec' % timer.stop())
```

Done in 0.0377 sec

Below, we use `waitall` as an example. The time output includes the calculation time of `y` and `z` respectively.

```
timer.start()
y = nd.dot(x, x)
z = nd.dot(x, x)
nd.waitall()
print('Done in %.4f sec' % timer.stop())
```

Done in 0.0735 sec

Additionally, any operation that does not support asynchronous programming but converts the NDArray into another data structure will cause the front-end to have to wait for computation results. For example, calling the `asnumpy` and `asscalar` functions:

```
timer.start()
y = nd.dot(x, x)
y.asnumpy()
print('Done in %.4f sec' % timer.stop())
```

Done in 0.0409 sec

```
timer.start()
y = nd.dot(x, x)
y.norm().asscalar()
print('Done in %.4f sec' % timer.stop())
```

Done in 0.1372 sec

The `wait_to_read`, `waitall`, `asnumpy`, `asscalar` and `theprint` functions described above will cause the front-end to wait for the back-end computation results. Such functions are often referred to as synchronization functions.

### 13.2.3 Using Asynchronous Programming to Improve Computing Performance

In the following example, we will use the “for” loop to continuously assign values to the variable `y`. Asynchronous programming is not used in tasks when the synchronization function `wait_to_read` is used in the “for” loop. However, when the synchronization function `waitall` is used outside of the “for” loop, asynchronous programming is used.

```
timer.start()
for _ in range(1000):
    y = x + 1
    y.wait_to_read()
print('Synchronous. Done in %.4f sec' % timer.stop())

timer.start()
for _ in range(1000):
    y = x + 1
nd.waitall()
print('Asynchronous. Done in %.4f sec' % timer.stop())
```

```
Synchronous. Done in 0.3632 sec
Asynchronous. Done in 0.1724 sec
```

We have observed that certain aspects of computing performance can be improved by making use of asynchronous programming. To explain this, we will slightly simplify the interaction between the Python front-end thread and the C++ back-end thread. In each loop, the interaction between front and back-ends can be largely divided into three stages:

1. The front-end orders the back-end to insert the calculation task  $y = x + 1$  into the queue.
2. The back-end then receives the computation tasks from the queue and performs the actual computations.
3. The back-end then returns the computation results to the front-end.

Assume that the durations of these three stages are  $t_1, t_2, t_3$ , respectively. If we do not use asynchronous programming, the total time taken to perform 1000 computations is approximately  $1000(t_1 + t_2 + t_3)$ . If asynchronous programming is used, the total time taken to perform 1000 computations can be reduced to  $t_1 + 1000t_2 + t_3$  (assuming  $1000t_2 > 999t_1$ ), since the front-end does not have to wait for the back-end to return computation results for each loop.

### 13.2.4 The Impact of Asynchronous Programming on Memory

In order to explain the impact of asynchronous programming on memory usage, recall what we learned in the previous chapters. Throughout the model training process implemented in the previous chapters, we usually evaluated things like the loss or accuracy of the model in each mini-batch. Detail-oriented readers may have discovered that such evaluations often make use of synchronization functions, such as `asscalar` or `asnumpy`. If these synchronization functions are removed, the front-end will pass a large number of mini-batch computing tasks to the back-end in a very short time, which might cause a spike in memory usage. When the mini-batches makes use of synchronization functions, on each iteration, the front-end will only pass one mini-batch task to the back-end to be computed, which will typically reduce memory use.

Because the deep learning model is usually large and memory resources are usually limited, we recommend the use of synchronization functions for each mini-batch throughout model training, for example by using the `asscalar` or `asnumpy` functions to evaluate model performance. Similarly, we also recommend utilizing synchronization functions for each mini-batch prediction (such as directly printing out the current batch's prediction results), in order to reduce memory usage during model prediction.

Next, we will demonstrate asynchronous programming's impact on memory. We will first define a data retrieval function `data_iter`, which upon being called, will start timing and regularly print out the time taken to retrieve data batches.

```
def data_iter():
    timer.start()
    num_batches, batch_size = 100, 1024
    for i in range(num_batches):
        X = nd.random.normal(shape=(batch_size, 512))
        y = nd.ones((batch_size,))
        yield X, y
        if (i + 1) % 50 == 0:
            print('batch %d, time %.4f sec' % (i + 1, timer.stop()))
```

The multilayer perceptron, optimization algorithm, and loss function are defined below.

```
net = nn.Sequential()
net.add(nn.Dense(2048, activation='relu'),
       nn.Dense(512, activation='relu'),
       nn.Dense(1))
net.initialize()
trainer = gluon.Trainer(net.collect_params(), 'sgd', {'learning_rate': 0.005})
loss = gluon.loss.L2Loss()
```

A helper function to monitor memory use is defined here. It should be noted that this function can only be run on Linux or MacOS operating systems.

```
def get_mem():
    res = subprocess.check_output(['ps', 'u', '-p', str(os.getpid())])
    return int(res.split()[15]) / 1e3
```

Now we can begin testing. To initialize the `net` parameters we will try running the system once. See Section 7.3 for further discussions related to initialization.

```
for X, y in data_iter():
    break
loss(y, net(X)).wait_to_read()
```

For the `net` training model, the synchronization function `asscalar` can naturally be used to record the loss of each mini-batch output by the NDArray format and to print out the model loss after each iteration. At this point, the generation interval of each mini-batch increases, but with a small memory overhead.

```
l_sum, mem = 0, get_mem()
for X, y in data_iter():
    with autograd.record():
        l = loss(y, net(X))
    # Use of the Asscalar synchronization function
    l_sum += l.mean().asscalar()
    l.backward()
    trainer.step(X.shape[0])
nd.waitall()
print('increased memory: %f MB' % (get_mem() - mem))
```

```
batch 50, time 2.2931 sec
batch 100, time 4.6425 sec
increased memory: 7.128000 MB
```

Even though each mini-batch's generation interval is shorter, the memory usage may still be high during

training if the synchronization function is removed. This is because, in default asynchronous programming, the front-end will pass on all mini-batch computations to the back-end in a short amount of time. As a result of this, a large amount of intermediate results cannot be released and may end up piled up in memory. In this experiment, we can see that all data ( $X$  and  $y$ ) is generated in under a second. However, because of an insufficient training speed, this data can only be stored in the memory and cannot be cleared in time, resulting in extra memory usage.

```
mem = get_mem()
for X, y in data_iter():
    with autograd.record():
        l = loss(y, net(X))
    l.backward()
    trainer.step(X.shape[0])
nd.waitall()
print('increased memory: %f MB' % (get_mem() - mem))
```

```
batch 50, time 0.0810 sec
batch 100, time 0.1610 sec
increased memory: 196.628000 MB
```

### 13.2.5 Summary

- MXNet includes the front-end used directly by users for interaction and the back-end used by the system to perform the computation.
- MXNet can improve computing performance through the use of asynchronous programming.
- We recommend using at least one synchronization function for each mini-batch training or prediction to avoid passing on too many computation tasks to the back-end in a short period of time.

### 13.2.6 Exercises

- In the section “Use of Asynchronous Programming to Improve Computing Performance”, we mentioned that using asynchronous computation can reduce the total amount of time needed to perform 1000 computations to  $t_1 + 1000t_2 + t_3$ . Why do we have to assume  $1000t_2 > 999t_1$  here?

### 13.2.7 Scan the QR Code to Discuss<sup>172</sup>



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<sup>172</sup> <https://discuss.mxnet.io/t/2381>

## 13.3 Automatic Parallelism

MXNet automatically constructs computational graphs at the back end. Using a computational graph, the system is aware of all the computational dependencies, and can selectively execute multiple non-interdependent tasks in parallel to improve computing performance. For instance, the first example in Section 13.2 executes `a = nd.ones((1, 2))` and `b = nd.ones((1, 2))` in turn. There is no dependency between these two steps, so the system can choose to execute them in parallel.

Typically, a single operator will use all the computational resources on all CPUs or a single GPU. For example, the `dot` operator will use all threads on all CPUs (even if there are multiple CPU processors on a single machine) or a single GPU. If computational load of each operator is large enough and multiple operators are run in parallel on only on the CPU or a single GPU, then the operations of each operator can only receive a portion of computational resources of CPU or single GPU. Even if these computations can be parallelized, the ultimate increase in computing performance may not be significant. In this section, our discussion of automatic parallel computation mainly focuses on parallel computation using both CPUs and GPUs, as well as the parallelization of computation and communication.

First, import the required packages or modules for experiment in this section. Note that we need at least one GPU to run the experiment in this section.

```
import d2l
from mxnet import nd, context
```

### 13.3.1 Parallel Computation using CPUs and GPUs

First, we will discuss parallel computation using CPUs and GPUs, for example, when computation in a program occurs both on the CPU and a GPU. First, define the `run` function so that it performs 10 matrix multiplications.

```
def run(x):
    return [nd.dot(x, x) for _ in range(10)]
```

Next, create an NDArray on both the CPU and GPU.

```
x_cpu = nd.random.uniform(shape=(2000, 2000))
x_gpu = nd.random.uniform(shape=(6000, 6000), ctx=d2l.try_gpu())
```

Then, use the two NDArrays to run the `run` function on both the CPU and GPU and print the time required.

```
run(x_cpu) # Warm-up begins
run(x_gpu)
nd.waitall() # Warm-up ends

timer = d2l.Timer()
run(x_cpu)
nd.waitall()
print('Run on %s: %.4f sec' % (x_cpu.context, timer.stop()))

timer.start()
run(x_gpu)
nd.waitall()
print('Run on %s: %.4f sec' % (x_gpu.context, timer.stop()))
```

```
Run on cpu(0): 0.3638 sec
Run on gpu(0): 0.3097 sec
```

We remove `nd.waitall()` between the two computing tasks `run(x_cpu)` and `run(x_gpu)` and hope the system can automatically parallel these two tasks.

```
timer.start()
run(x_cpu)
run(x_gpu)
nd.waitall()
print('Run on both %s and %s: %.4f sec' % (
    x_cpu.context, x_gpu.context, timer.stop()))
```

```
Run on both cpu(0) and gpu(0): 0.3639 sec
```

As we can see, when two computing tasks are executed together, the total execution time is less than the sum of their separate execution times. This means that MXNet can effectively automate parallel computation on CPUs and GPUs.

### 13.3.2 Parallel Computation of Computing and Communication

In computations that use both the CPU and GPU, we often need to copy data between the CPU and GPU, resulting in data communication. In the example below, we compute on the GPU and then copy the results back to the CPU. We print the GPU computation time and the communication time from the GPU to CPU.

```
def copy_to_cpu(x):
    return [y.copyto(context.cpu()) for y in x]

timer.start()
y = run(x_gpu)
nd.waitall()
print('Run on %s: %.4f sec' % (x_gpu.context, timer.stop()))

timer.start()
y_cpu = copy_to_cpu(y)
nd.waitall()
print('The copy to %s: %.4f sec' % (y_cpu[0].context, timer.stop()))
```

```
Run on gpu(0): 0.3141 sec
The copy to cpu(0): 0.5236 sec
```

We remove the `waitall` function between computation and communication and print the total time need to complete both tasks.

```
timer.start()
y = run(x_gpu)
y_cpu = copy_to_cpu(y)
nd.waitall()
print('Run and copy in parallel: %.4f sec' % timer.stop())
```

```
Run and copy in parallel: 0.5511 sec
```

As we can see, the total time required to perform computation and communication is less than the sum of their separate execution times. It should be noted that this computation and communication task is different from the parallel computation task that simultaneously used the CPU and GPU described earlier in this section. Here, there is a dependency between execution and communication:  $y[i]$  must be computed before it can be copied to the CPU. Fortunately, the system can copy  $y[i-1]$  when computing  $y[i]$  to reduce the total running time of computation and communication.

### 13.3.3 Summary

- MXNet can improve computing performance through automatic parallel computation, such as parallel computation using the CPU and GPU and the parallelization of computation and communication.

### 13.3.4 Exercises

- 10 operations were performed in the `run` function defined in this section. There are no dependencies between them. Design an experiment to see if MXNet will automatically execute them in parallel.
- Designing computation tasks that include more complex data dependencies, and run experiments to see if MXNet can obtain the correct results and improve computing performance.
- When the computational load of an operator is small enough, parallel computation on only the CPU or a single GPU may also improve the computing performance. Design an experiment to verify this.

### 13.3.5 Scan the QR Code to Discuss<sup>173</sup>



## 13.4 Multi-GPU Computation Implementation from Scratch

In this section, we will show how to use multiple GPU for computation. For example, we can train the same model using multiple GPUs. As you might expect, running the programs in this section requires at least two GPUs. In fact, installing multiple GPUs on a single machine is common because there are usually multiple PCIe slots on the motherboard. If the NVIDIA driver is properly installed, we can use the `nvidia-smi` command to view all GPUs on the current computer.

```
!nvidia-smi
```

```
Fri Jul 19 02:04:57 2019
```

NVIDIA-SMI 418.67	Driver Version: 418.67	CUDA Version: 10.1
GPU Name	Persistence-M  Bus-Id	Disp.A   Volatile Uncorr. ECC

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<sup>173</sup> <https://discuss.mxnet.io/t/2382>

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Fan	Temp	Perf	Pwr:Usage/Cap	Memory-Usage	GPU-Util	Compute M.
0	Tesla V100-SXM2...	Off	00000000:00:1B.0	Off		0
N/A	42C	P0	52W / 300W	0MiB / 16130MiB	0%	Default
+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+
1	Tesla V100-SXM2...	Off	00000000:00:1C.0	Off		0
N/A	42C	P0	54W / 300W	5895MiB / 16130MiB	0%	Default
+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+
2	Tesla V100-SXM2...	Off	00000000:00:1D.0	Off		0
N/A	55C	P0	242W / 300W	3356MiB / 16130MiB	76%	Default
+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+
3	Tesla V100-SXM2...	Off	00000000:00:1E.0	Off		0
N/A	44C	P0	55W / 300W	1038MiB / 16130MiB	0%	Default
+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+
Processes:				GPU Memory		
GPU	PID	Type	Process name	Usage		
+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+
1	49887	C	/home/ubuntu/miniconda3/bin/python	1001MiB		
1	53467	C	/home/ubuntu/miniconda3/bin/python	1133MiB		
1	59096	C	/home/ubuntu/miniconda3/bin/python	993MiB		
1	108923	C	/home/ubuntu/miniconda3/bin/python	2757MiB		
2	33304	C	...ins/miniconda3/envs/d2l-en-1/bin/python	3345MiB		
3	53467	C	/home/ubuntu/miniconda3/bin/python	1027MiB		
+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+	+-----+-----+-----+-----+-----+-----+-----+

As we discussed in Section 13.3, most operations can use all the computational resources of all CPUs, or all computational resources of a single GPU. However, if we use multiple GPUs for model training, we still need to implement the corresponding algorithms. Of these, the most commonly used algorithm is called data parallelism.

### 13.4.1 Data Parallelism

In the deep learning field, Data Parallelism is currently the most widely used method for dividing model training tasks among multiple GPUs. Recall the process for training models using optimization algorithms described in Section 12.5. Now, we will demonstrate how data parallelism works using mini-batch stochastic gradient descent as an example.

Assume there are  $k$  GPUs on a machine. Given the model to be trained, each GPU will maintain a complete set of model parameters independently. In any iteration of model training, given a random mini-batch, we divide the examples in the batch into  $k$  portions and distribute one to each GPU. Then, each GPU will calculate the local gradient of the model parameters based on the mini-batch subset it was assigned and the model parameters it maintains. Next, we add together the local gradients on the  $k$  GPUs to get the current mini-batch stochastic gradient. After that, each GPU uses this mini-batch stochastic gradient to update the complete set of model parameters that it maintains. Figure 10.1 depicts the mini-batch stochastic gradient calculation using data parallelism and two GPUs.

In order to implement data parallelism in a multi-GPU training scenario from scratch, we first import the required packages or modules.

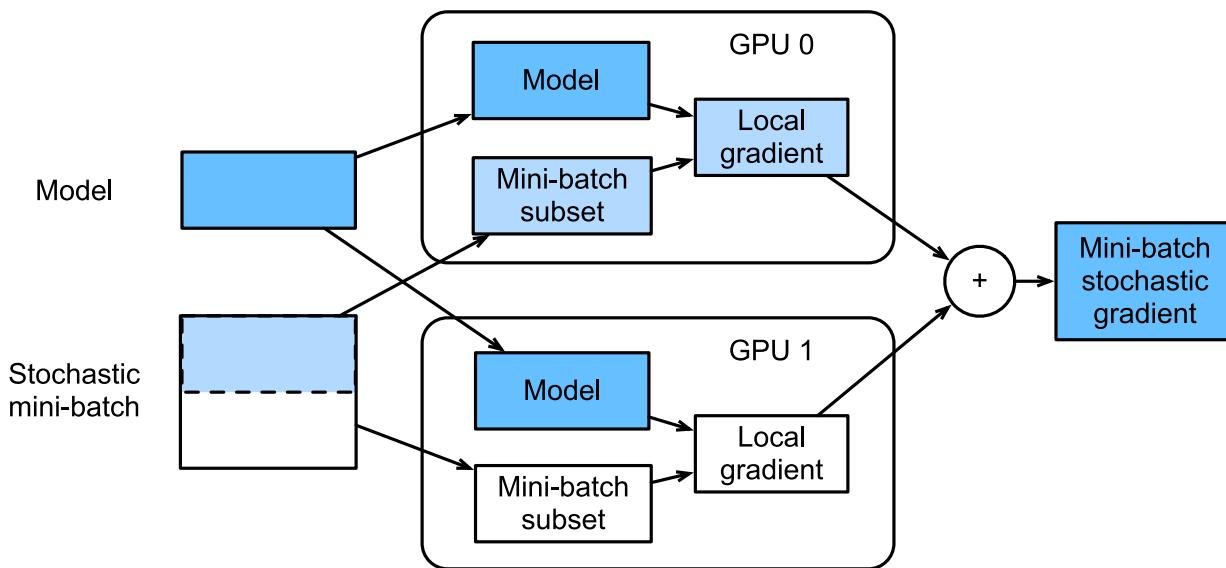


Fig. 13.4.1: Calculation of mini-batch stochastic gradient using data parallelism and two GPUs.

```
%matplotlib inline
import d2l
from mxnet import autograd, nd, gluon
```

### 13.4.2 Define the Model

We use LeNet, introduced in Section 8.6, as the sample model for this section. Here, the model implementation only uses NDArray.

```
# Initialize model parameters
scale = 0.01
W1 = nd.random.normal(scale=scale, shape=(20, 1, 3, 3))
b1 = nd.zeros(shape=20)
W2 = nd.random.normal(scale=scale, shape=(50, 20, 5, 5))
b2 = nd.zeros(shape=50)
W3 = nd.random.normal(scale=scale, shape=(800, 128))
b3 = nd.zeros(shape=128)
W4 = nd.random.normal(scale=scale, shape=(128, 10))
b4 = nd.zeros(shape=10)
params = [W1, b1, W2, b2, W3, b3, W4, b4]

# Define the model
def lenet(X, params):
    h1_conv = nd.Convolution(data=X, weight=params[0], bias=params[1],
                            kernel=(3, 3), num_filter=20)
    h1_activation = nd.relu(h1_conv)
    h1 = nd.Pooling(data=h1_activation, pool_type='avg', kernel=(2, 2),
                    stride=(2, 2))
    h2_conv = nd.Convolution(data=h1, weight=params[2], bias=params[3],
                            kernel=(5, 5), num_filter=50)
```

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```

h2_activation = nd.relu(h2_conv)
h2 = nd.Pooling(data=h2_activation, pool_type='avg', kernel=(2, 2),
                 stride=(2, 2))
h2 = nd.flatten(h2)
h3_linear = nd.dot(h2, params[4]) + params[5]
h3 = nd.relu(h3_linear)
y_hat = nd.dot(h3, params[6]) + params[7]
return y_hat

# Cross-entropy loss function
loss = gluon.loss.SoftmaxCrossEntropyLoss()

```

### 13.4.3 Synchronize Data Among Multiple GPUs

We need to implement some auxiliary functions to synchronize data among the multiple GPUs. The following `get_params` function copies the model parameters to a specific GPU and initializes the gradient.

```

def get_params(params, ctx):
    new_params = [p.copyto(ctx) for p in params]
    for p in new_params:
        p.attach_grad()
    return new_params

```

Try to copy the model parameter `params` to `gpu(0)`.

```

new_params = get_params(params, d2l.try_gpu(0))
print('b1 weight:', new_params[1])
print('b1 grad:', new_params[1].grad)

```

```

b1 weight:
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
<NDArray 20 @gpu(0)>
b1 grad:
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
<NDArray 20 @gpu(0)>

```

Here, the data is distributed among multiple GPUs. The following `allreduce` function adds up the data on each GPU and then broadcasts it to all the GPUs.

```

def allreduce(data):
    for i in range(1, len(data)):
        data[0][:] += data[i].copyto(data[0].context)
    for i in range(1, len(data)):
        data[0].copyto(data[i])

```

Perform a simple test of the `allreduce` function.

```

data = [nd.ones((1, 2), ctx=d2l.try_gpu(i)) * (i + 1) for i in range(2)]
print('before allreduce:', data)
allreduce(data)
print('after allreduce:', data)

```

```
before allreduce: [
[[1. 1.]]
<NDArray 1x2 @gpu(0)>,
[[2. 2.]]
<NDArray 1x2 @gpu(1)>
after allreduce: [
[[3. 3.]]
<NDArray 1x2 @gpu(0)>,
[[3. 3.]]
<NDArray 1x2 @gpu(1)>]
```

### 13.4.4 Split a Data Batch into Multiple GPUs

The `utils` module in Gluon provides a function to evenly split an array into multiple parts along the first dimension, and then copy the  $i$ -th part into the  $i$ -th device. It's straightforward to implement, but we will use the pre-implemented version so later chapters can reuse the `split_batch` function we will define later.

Now, we try to divide the 6 data instances equally between 2 GPUs using the `split_and_load` function.

```
data = nd.arange(24).reshape((6, 4))
ctx = d2l.try_all_gpus()
splitted = gluon.utils.split_and_load(data, ctx)
print('input: ', data)
print('load into', ctx)
print('output:', splitted)
```

```
input:
[[ 0.  1.  2.  3.]
 [ 4.  5.  6.  7.]
 [ 8.  9. 10. 11.]
 [12. 13. 14. 15.]
 [16. 17. 18. 19.]
 [20. 21. 22. 23.]]
<NDArray 6x4 @cpu(0)>
load into [gpu(0), gpu(1)]
output:
[[ 0.  1.  2.  3.]
 [ 4.  5.  6.  7.]
 [ 8.  9. 10. 11.]]
<NDArray 3x4 @gpu(0)>,
[[12. 13. 14. 15.]
 [16. 17. 18. 19.]
 [20. 21. 22. 23.]]
<NDArray 3x4 @gpu(1)>]
```

The `split_batch` function then splits both the features and labels.

```
# Save to the d2l package.
def split_batch(X, y, ctx_list):
    """Split X and y into multiple devices specified by ctx"""
    assert X.shape[0] == y.shape[0]
```

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```
return (gluon.utils.split_and_load(X, ctx_list),
       gluon.utils.split_and_load(y, ctx_list))
```

### 13.4.5 Multi-GPU Training on a Single Mini-batch

Now we can implement multi-GPU training on a single mini-batch. Its implementation is primarily based on the data parallelism approach described in this section. We will use the auxiliary functions we just discussed, `allreduce` and `split_and_load`, to synchronize the data among multiple GPUs.

```
def train_batch(X, y, gpu_params, ctx_list, lr):
    gpu_Xs, gpu_ys = split_batch(X, y, ctx_list)
    with autograd.record(): # Loss is calculated separately on each GPU
        ls = [loss(lenet(gpu_X, gpu_W), gpu_y)
              for gpu_X, gpu_y, gpu_W in zip(gpu_Xs, gpu_ys, gpu_params)]
    for l in ls: # Back Propagation is performed separately on each GPU
        l.backward()
    # Add up all the gradients from each GPU and then broadcast them to all
    # the GPUs
    for i in range(len(gpu_params[0])):
        allreduce([gpu_params[c][i].grad for c in range(len(ctx_list))])
    # The model parameters are updated separately on each GPU
    for param in gpu_params:
        d2l.sgd(param, lr, X.shape[0]) # Here, we use a full-size batch
```

### 13.4.6 Training Functions

Now, we can define the training function. Here the training function is slightly different from the one used in the previous chapter. For example, here, we need to copy all the model parameters to multiple GPUs based on data parallelism and perform multi-GPU training on a single mini-batch for each iteration.

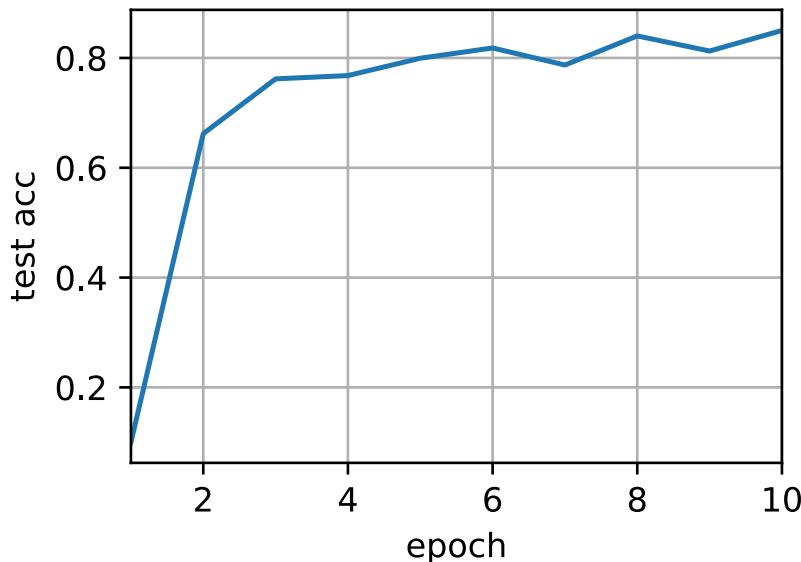
```
def train(num_gpus, batch_size, lr):
    train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size)
    ctx_list = [d2l.try_gpu(i) for i in range(num_gpus)]
    # Copy model parameters to num_gpus GPUs
    gpu_params = [get_params(params, c) for c in ctx_list]
    num_epochs, times, acces = 10, [], []
    animator = d2l.Animator('epoch', 'test acc', xlim=[1, num_epochs])
    timer = d2l.Timer()
    for epoch in range(num_epochs):
        timer.start()
        for X, y in train_iter:
            # Perform multi-GPU training for a single mini-batch
            train_batch(X, y, gpu_params, ctx_list, lr)
            nd.waitall()
        timer.stop()
        # Verify the model on GPU 0
        animator.add(epoch+1, d2l.evaluate_accuracy_gpu(
            lambda x: lenet(x, gpu_params[0]), test_iter, ctx[0]))
    print('test acc: %.2f, %.1f sec/epoch on %s' %
          (animator.Y[0][-1], timer.avg(), ctx_list))
```

### 13.4.7 Multi-GPU Training Experiment

We will start by training with a single GPU. Assume the batch size is 256 and the learning rate is 0.2.

```
train(num_gpus=1, batch_size=256, lr=0.2)
```

```
test acc: 0.85, 1.5 sec/epoch on [gpu(0)]
```

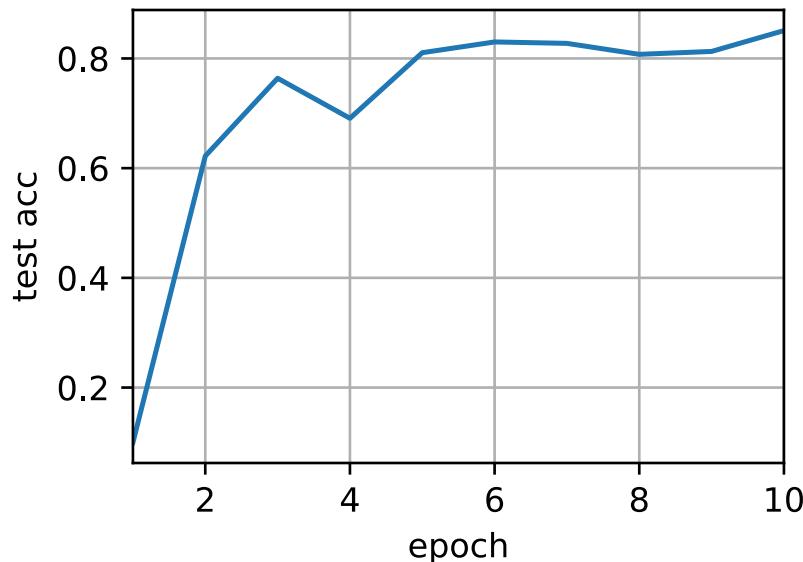


By keeping the batch size and learning rate unchanged and changing the number of GPUs to 2, we can see that the improvement in test accuracy is roughly the same as in the results from the previous experiment. In terms of the optimization algorithms, they are identical.

Because of the extra communication overhead, and relative simple model we used here, there is no reduction in the training time. We will consider a more complex model in the next chapter.

```
train(num_gpus=2, batch_size=256, lr=0.2)
```

```
test acc: 0.85, 2.4 sec/epoch on [gpu(0), gpu(1)]
```



### 13.4.8 Summary

- We can use data parallelism to more fully utilize the computational resources of multiple GPUs to implement multi-GPU model training.
- With the same hyper-parameters, the training accuracy of the model is roughly equivalent when we change the number of GPUs.

### 13.4.9 Exercises

- In a multi-GPU training experiment, use 2 GPUs for training and double the `batch_size` to 512. How does the training time change? If we want a test accuracy comparable with the results of single-GPU training, how should the learning rate be adjusted?
- Change the model prediction part of the experiment to multi-GPU prediction.

### 13.4.10 Scan the QR Code to Discuss<sup>174</sup>



## 13.5 Concise Implementation of Multi-GPU Computation

In Gluon, we can conveniently use data parallelism to perform multi-GPU computation. For example, we do not need to implement the helper function to synchronize data among multiple GPUs, as described in

<sup>174</sup> <https://discuss.mxnet.io/t/2383>

Section 13.4, ourselves.

First, import the required packages or modules for the experiment in this section. Running the programs in this section requires at least two GPUs.

```
import d2l
from mxnet import autograd, gluon, init, nd
from mxnet.gluon import nn
```

### 13.5.1 Initialize Model Parameters on Multiple GPUs

In this section, we use ResNet-18 as a sample model. Since the input images in this section are original size (not enlarged), the model construction here is different from the ResNet-18 structure described in Section 9.6. This model uses a smaller convolution kernel, stride, and padding at the beginning and removes the maximum pooling layer.

```
# Save to the d2l package.
def resnet18(num_classes):
    """A slightly modified ResNet-18 model"""
    def resnet_block(num_channels, num_residuals, first_block=False):
        blk = nn.Sequential()
        for i in range(num_residuals):
            if i == 0 and not first_block:
                blk.add(d2l.Residual(
                    num_channels, use_1x1conv=True, strides=2))
            else:
                blk.add(d2l.Residual(num_channels))
        return blk

    net = nn.Sequential()
    # This model uses a smaller convolution kernel, stride, and padding and
    # removes the maximum pooling layer
    net.add(nn.Conv2D(64, kernel_size=3, strides=1, padding=1),
            nn.BatchNorm(), nn.Activation('relu'))
    net.add(resnet_block(64, 2, first_block=True),
            resnet_block(128, 2),
            resnet_block(256, 2),
            resnet_block(512, 2))
    net.add(nn.GlobalAvgPool2D(), nn.Dense(num_classes))
    return net

net = resnet18(10)
```

Previously, we discussed how to use the `initialize` function's `ctx` parameter to initialize model parameters on a CPU or a single GPU. In fact, `ctx` can accept a range of CPUs and GPUs so as to copy initialized model parameters to all CPUs and GPUs in `ctx`.

```
ctx = d2l.try_all_gpus()
net.initialize(init=init.Normal(sigma=0.01), ctx=ctx)
```

Gluon provides the `split_and_load` function implemented in the previous section. It can divide a mini-batch of data instances and copy them to each CPU or GPU. Then, the model computation for the data input to each CPU or GPU occurs on that same CPU or GPU.

```
x = nd.random.uniform(shape=(4, 1, 28, 28))
gpu_x = gluon.utils.split_and_load(x, ctx)
net(gpu_x[0]), net(gpu_x[1])
```

```
(  
[[ 5.48149364e-06 -8.33710089e-07 -1.63167692e-06 -6.36740765e-07  
-3.82161761e-06 -2.35140669e-06 -2.54695851e-06 -9.47824219e-08  
-6.90335582e-07 2.57562374e-06]  
[ 5.47108630e-06 -9.42463600e-07 -1.04940591e-06 9.80820687e-08  
-3.32518266e-06 -2.48629135e-06 -3.36428002e-06 1.04560286e-07  
-6.10012194e-07 2.03278501e-06]  
<NDArray 2x10 @gpu(0)>,  
[[ 5.6176350e-06 -1.2837600e-06 -1.4605525e-06 1.8302978e-07  
-3.5511648e-06 -2.4371018e-06 -3.5731791e-06 -3.0974837e-07  
-1.1016566e-06 1.8909888e-06]  
[ 5.1418701e-06 -1.3729926e-06 -1.1520079e-06 1.1507450e-07  
-3.7372806e-06 -2.8289705e-06 -3.6477188e-06 1.5781586e-07  
-6.0733169e-07 1.9712008e-06]  
<NDArray 2x10 @gpu(1)>)
```

Now we can access the initialized model parameter values through `data`. It should be noted that `weight.data()` will return the parameter values on the CPU by default. Since we specified 2 GPUs to initialize the model parameters, we need to specify the GPU to access parameter values. As we can see, the same parameters have the same values on different GPUs.

```
weight = net[0].params.get('weight')

try:
    weight.data()
except RuntimeError:
    print('not initialized on cpu')
weight.data(ctx[0])[0], weight.data(ctx[1])[0]
```

```
not initialized on cpu
```

```
(  
[[[-0.01473444 -0.01073093 -0.01042483]
[-0.01327885 -0.01474966 -0.00524142]
[ 0.01266256  0.00895064 -0.00601594]]]
<NDArray 1x3x3 @gpu(0)>,
[[[-0.01473444 -0.01073093 -0.01042483]
[-0.01327885 -0.01474966 -0.00524142]
[ 0.01266256  0.00895064 -0.00601594]]]
<NDArray 1x3x3 @gpu(1)>)
```

Remember we define the `evaluate_accuracy_gpu` in Section 8.6 to support evaluating on a single GPU, now we refine this implementation to support multiple devices.

```
# Save to the d2l package.
def evaluate_accuracy_gpus(net, data_iter):
    # Query the list of devices.
    ctx_list = list(net.collect_params().values())[0].list_ctx()
```

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```

metric = d2l.Accumulator(2) # num_corrected_examples, num_examples
for features, labels in data_iter:
    Xs, ys = d2l.split_batch(features, labels, ctx_list)
    pys = [net(X) for X in Xs] # run in parallel
    metric.add(sum(d2l.accuracy(py, y) for py, y in zip(pys, ys)),
               labels.size)
return metric[0]/metric[1]

```

### 13.5.2 Multi-GPU Model Training

When we use multiple GPUs to train the model, the `Trainer` instance will automatically perform data parallelism, such as dividing mini-batches of data instances and copying them to individual GPUs and summing the gradients of each GPU and broadcasting the result to all GPUs. In this way, we can easily implement the training function.

```

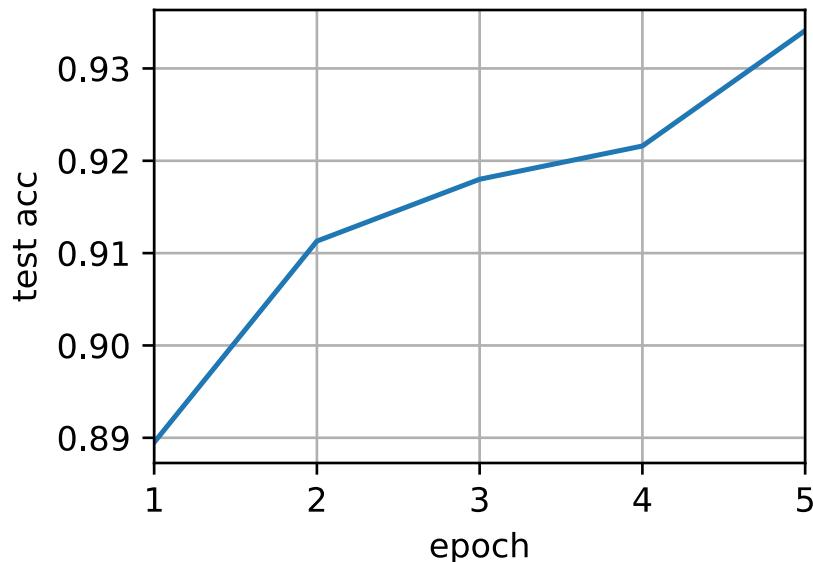
def train(num_gpus, batch_size, lr):
    train_iter, test_iter = d2l.load_data_fashion_mnist(batch_size)
    ctx_list = [d2l.try_gpu(i) for i in range(num_gpus)]
    net.initialize(init=init.Normal(sigma=0.01),
                   ctx=ctx_list, force_reinit=True)
    trainer = gluon.Trainer(
        net.collect_params(), 'sgd', {'learning_rate': lr})
    loss = gluon.loss.SoftmaxCrossEntropyLoss()
    timer, num_epochs = d2l.Timer(), 5
    animator = d2l.Animator('epoch', 'test acc', xlim=[1, num_epochs])
    for epoch in range(num_epochs):
        timer.start()
        for features, labels in train_iter:
            Xs, ys = d2l.split_batch(features, labels, ctx_list)
            with autograd.record():
                ls = [loss(net(X), y) for X, y in zip(Xs, ys)]
            for l in ls:
                l.backward()
            trainer.step(batch_size)
            nd.waitall()
            timer.stop()
            animator.add(epoch+1, evaluate_accuracy_gpus(net, test_iter))
        print('test acc: %.2f, %.1f sec/epoch on %s' %
              (animator.Y[0][-1], timer.avg(), ctx_list))

```

First, use a single GPU for training.

```
train(num_gpus=1, batch_size=256, lr=0.1)
```

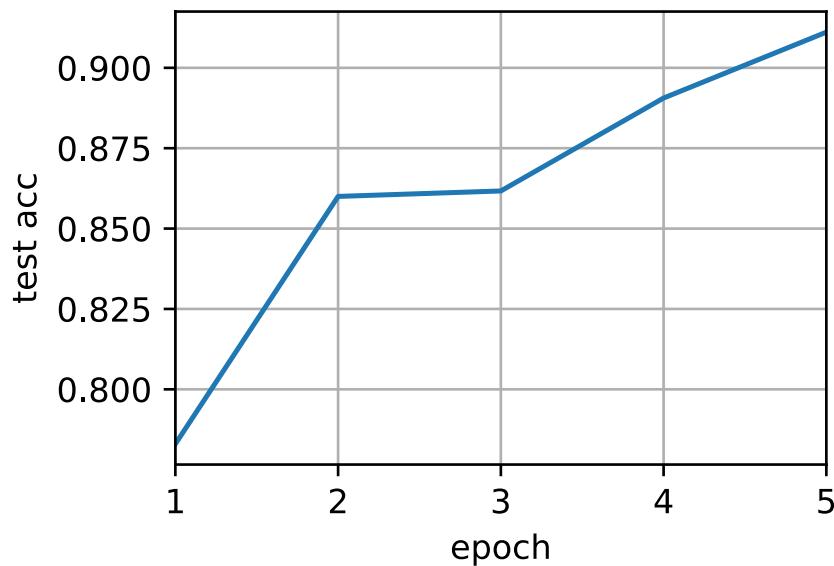
```
test acc: 0.93, 13.5 sec/epoch on [gpu(0)]
```



Then we try to use 2 GPUs for training. Compared with the LeNet used in the previous section, ResNet-18 computing is more complicated and the communication time is shorter compared to the calculation time, so parallel computing in ResNet-18 better improves performance.

```
train(num_gpus=2, batch_size=512, lr=0.2)
```

```
test acc: 0.91, 7.0 sec/epoch on [gpu(0), gpu(1)]
```



### 13.5.3 Summary

- In Gluon, we can conveniently perform multi-GPU computations, such as initializing model parameters and training models on multiple GPUs.

### 13.5.4 Exercises

- This section uses ResNet-18. Try different epochs, batch sizes, and learning rates. Use more GPUs for computation if conditions permit.
- Sometimes, different devices provide different computing power. Some can use CPUs and GPUs at the same time, or GPUs of different models. How should we divide mini-batches among different CPUs or GPUs?

### 13.5.5 Scan the QR Code to Discuss<sup>175</sup>



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<sup>175</sup> <https://discuss.mxnet.io/t/2384>



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CHAPTER  
FOURTEEN

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## COMPUTER VISION

Many applications in the area of computer vision are closely related to our daily lives, now and in the future, whether medical diagnostics, driverless vehicles, camera monitoring, or smart filters. In recent years, deep learning technology has greatly enhanced computer vision systems' performance. It can be said that the most advanced computer vision applications are nearly inseparable from deep learning.

We have introduced deep learning models commonly used in the area of computer vision in the chapter "Convolutional Neural Networks" and have practiced simple image classification tasks. In this chapter, we will introduce image augmentation and fine tuning methods and apply them to image classification. Then, we will explore various methods of object detection. After that, we will learn how to use fully convolutional networks to perform semantic segmentation on images. Then, we explain how to use style transfer technology to generate images that look like the cover of this book. Finally, we will perform practice exercises on two important computer vision data sets to review the content of this chapter and the previous chapters.

### 14.1 Image Augmentation

We mentioned that large-scale data sets are prerequisites for the successful application of deep neural networks in [Section 9.1](#). Image augmentation technology expands the scale of training data sets by making a series of random changes to the training images to produce similar, but different, training examples. Another way to explain image augmentation is that randomly changing training examples can reduce a model's dependence on certain properties, thereby improving its capability for generalization. For example, we can crop the images in different ways, so that the objects of interest appear in different positions, reducing the model's dependence on the position where objects appear. We can also adjust the brightness, color, and other factors to reduce model's sensitivity to color. It can be said that image augmentation technology contributed greatly to the success of AlexNet. In this section we will discuss this technology, which is widely used in computer vision.

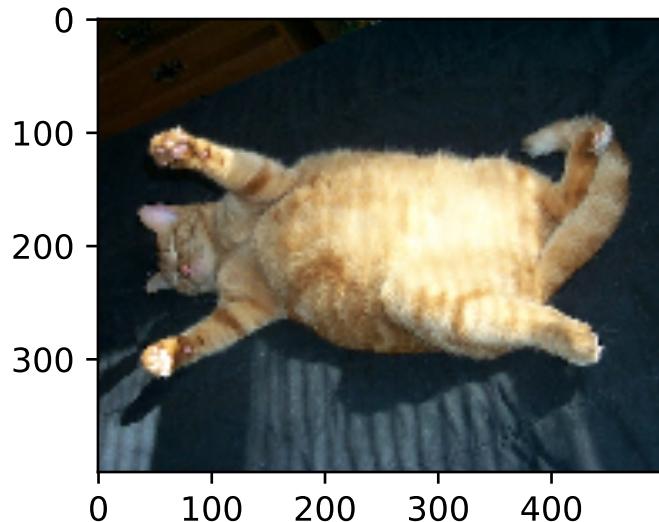
First, import the packages or modules required for the experiment in this section.

```
%matplotlib inline
import d2l
from mxnet import autograd, gluon, image, init, nd
from mxnet.gluon import nn
```

#### 14.1.1 Common Image Augmentation Method

In this experiment, we will use an image with a shape of  $400 \times 500$  as an example.

```
d2l.set_figsize((3.5, 2.5))
img = image.imread('../img/cat1.jpg')
d2l.plt.imshow(img.asnumpy());
```



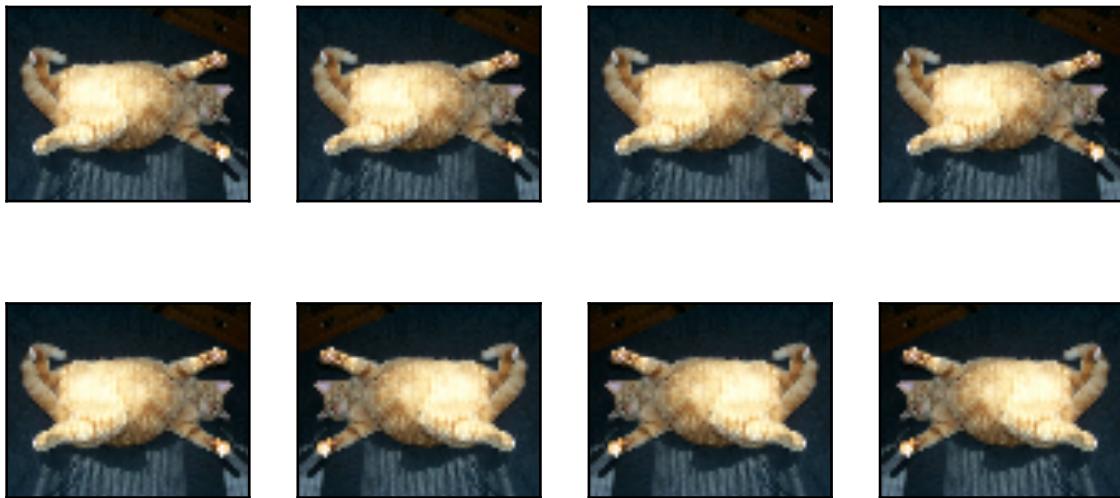
Most image augmentation methods have a certain degree of randomness. To make it easier for us to observe the effect of image augmentation, we next define the auxiliary function `apply`. This function runs the image augmentation method `aug` multiple times on the input image `img` and shows all results.

```
def apply(img, aug, num_rows=2, num_cols=4, scale=1.5):
    Y = [aug(img) for _ in range(num_rows * num_cols)]
    d2l.show_images(Y, num_rows, num_cols, scale=scale)
```

### Flip and Crop

Flipping the image left and right usually does not change the category of the object. This is one of the earliest and most widely used methods of image augmentation. Next, we use the `transforms` module to create the `RandomFlipLeftRight` instance, which introduces a 50% chance that the image is flipped left and right.

```
apply(img, gluon.data.vision.transforms.RandomFlipLeftRight())
```



Flipping up and down is not as commonly used as flipping left and right. However, at least for this example image, flipping up and down does not hinder recognition. Next, we create a `RandomFlipTopBottom` instance for a 50% chance of flipping the image up and down.

```
apply(img, gluon.data.vision.transforms.RandomFlipTopBottom())
```



In the example image we used, the cat is in the middle of the image, but this may not be the case for all images. In Section 8.5, we explained that the pooling layer can reduce the sensitivity of the convolutional layer to the target location. In addition, we can make objects appear at different positions in the image in different proportions by randomly cropping the image. This can also reduce the sensitivity of the model to the target position.

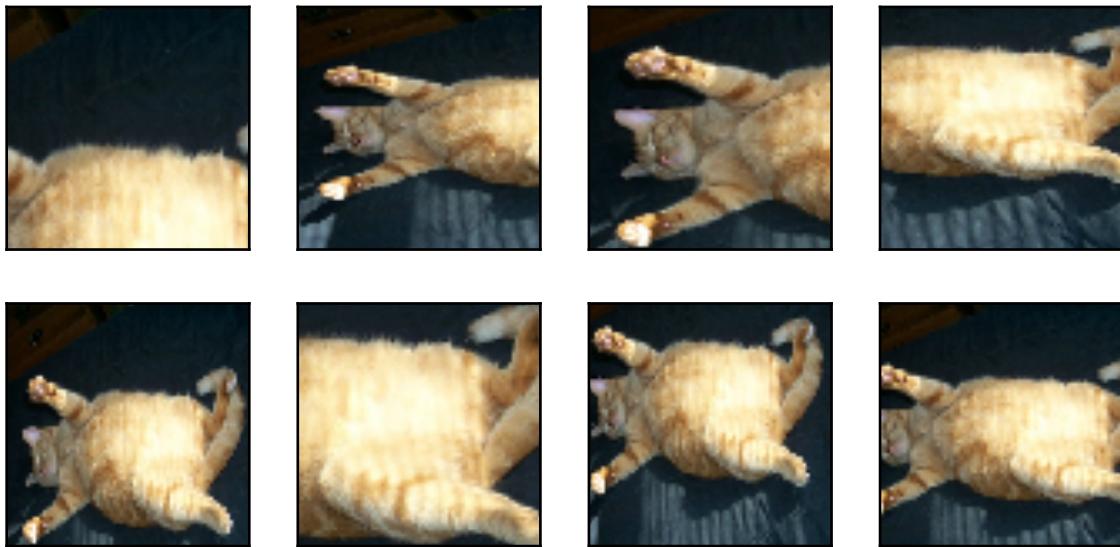
In the following code, we randomly crop a region with an area of 10% to 100% of the original area, and the ratio of width to height of the region is randomly selected from between 0.5 and 2. Then, the width and height of the region are both scaled to 200 pixels. Unless otherwise stated, the random number between  $a$  and  $b$  in this section refers to a continuous value obtained by uniform sampling in the interval  $[a, b]$ .

```
shape_aug = gluon.data.vision.transforms.RandomResizedCrop(
```

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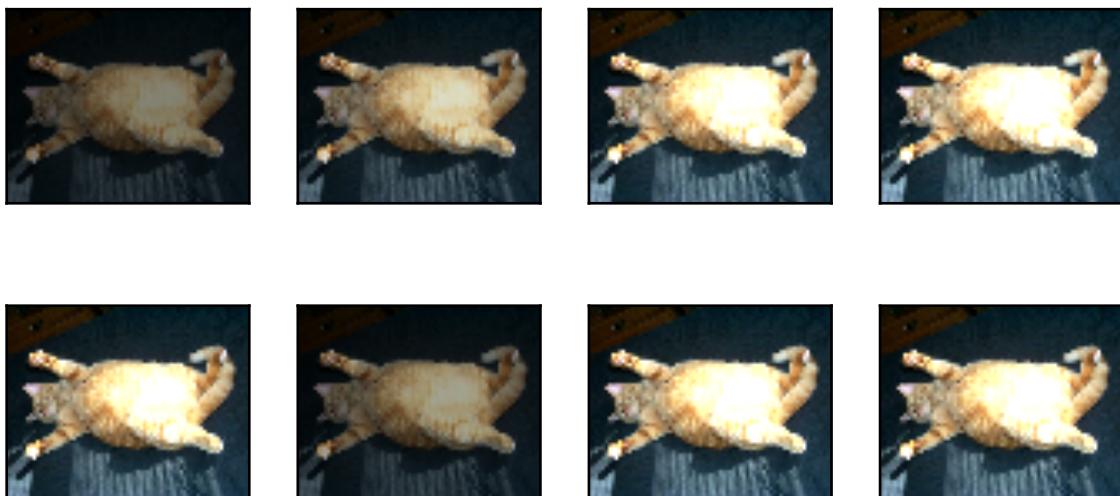
```
(200, 200), scale=(0.1, 1), ratio=(0.5, 2))  
apply(img, shape_aug)
```



### Change Color

Another augmentation method is changing colors. We can change four aspects of the image color: brightness, contrast, saturation, and hue. In the example below, we randomly change the brightness of the image to a value between 50% ( $1 - 0.5$ ) and 150% ( $1 + 0.5$ ) of the original image.

```
apply(img, gluon.data.vision.transforms.RandomBrightness(0.5))
```



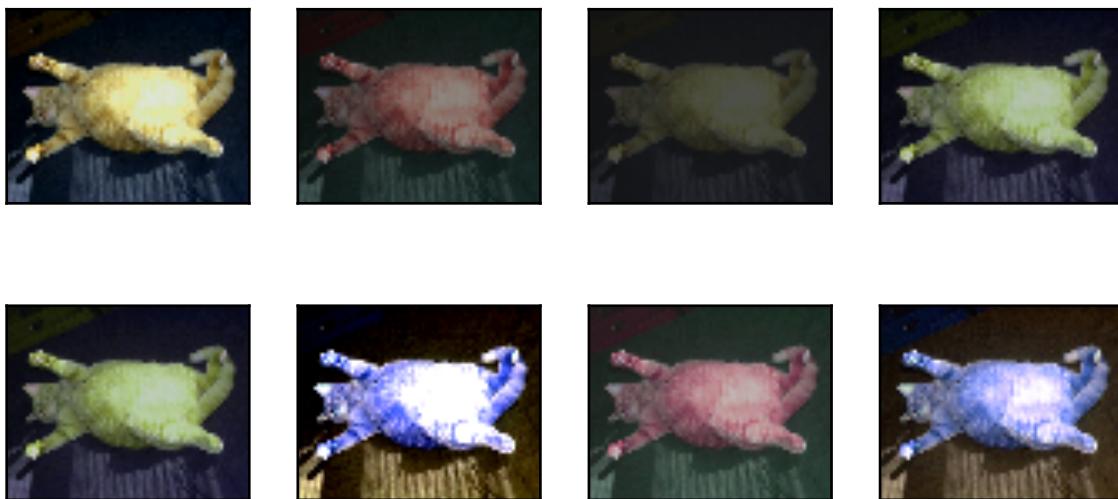
Similarly, we can randomly change the hue of the image.

```
apply(img, gluon.data.vision.transforms.RandomHue(0.5))
```



We can also create a `RandomColorJitter` instance and set how to randomly change the brightness, contrast, saturation, and hue of the image at the same time.

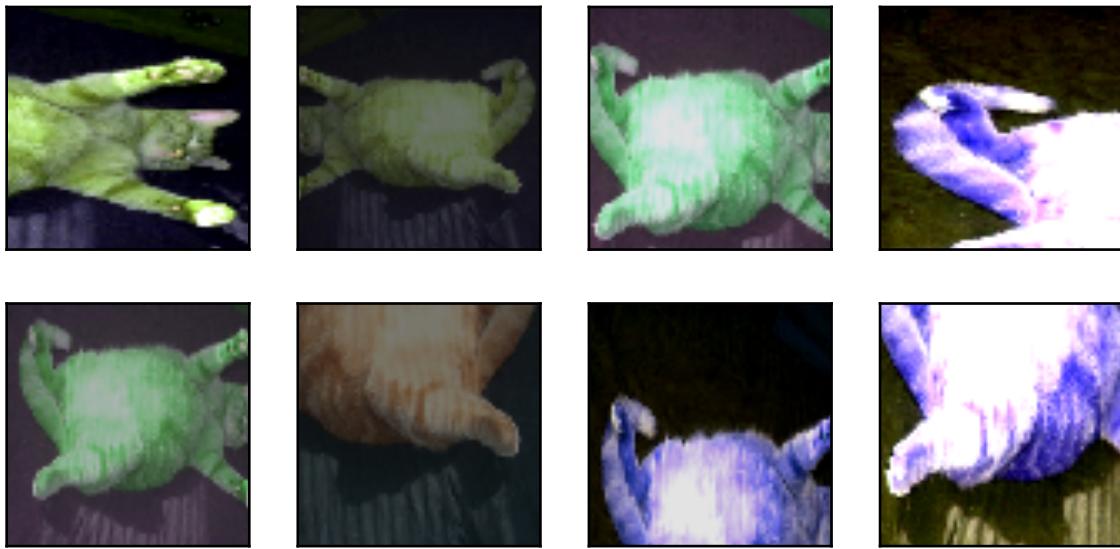
```
color_aug = gluon.data.vision.transforms.RandomColorJitter(
    brightness=0.5, contrast=0.5, saturation=0.5, hue=0.5)
apply(img, color_aug)
```



### Overlying Multiple Image Augmentation Methods

In practice, we will overlay multiple image augmentation methods. We can overlay the different image augmentation methods defined above and apply them to each image by using a `Compose` instance.

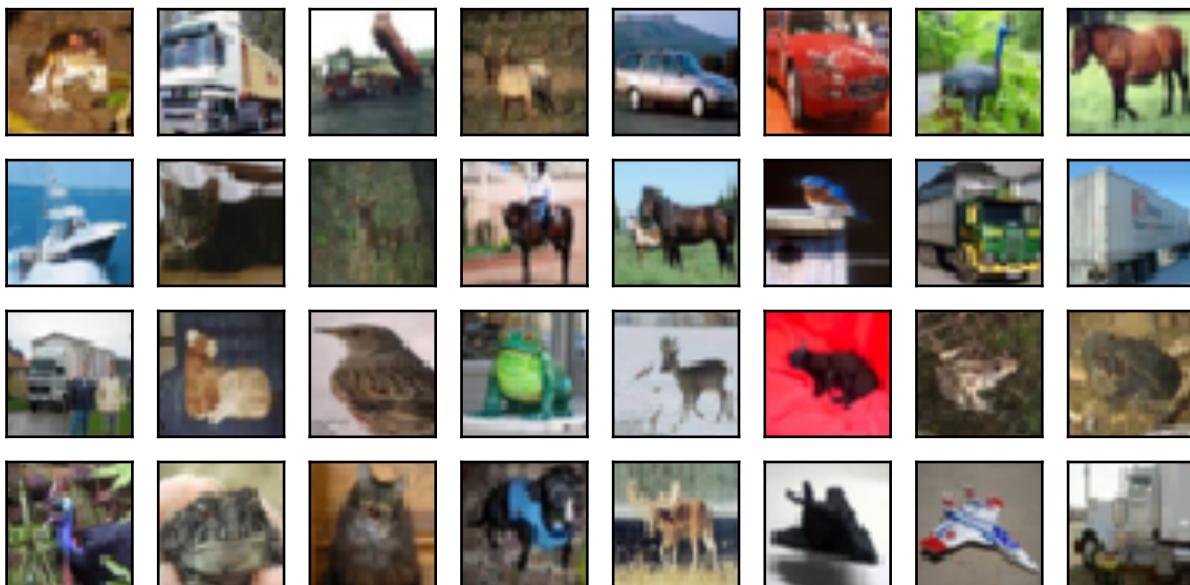
```
augs = gluon.data.vision.transforms.Compose([
    gluon.data.vision.transforms.RandomFlipLeftRight(), color_aug, shape_aug])
apply(img, augs)
```



### 14.1.2 Using an Image Augmentation Training Model

Next, we will look at how to apply image augmentation in actual training. Here, we use the CIFAR-10 data set, instead of the Fashion-MNIST data set we have been using. This is because the position and size of the objects in the Fashion-MNIST data set have been normalized, and the differences in color and size of the objects in CIFAR-10 data set are more significant. The first 32 training images in the CIFAR-10 data set are shown below.

```
d2l.show_images(gluon.data.vision.CIFAR10(  
    train=True)[0:32][0], 4, 8, scale=0.8);
```



In order to obtain a definitive results during prediction, we usually only apply image augmentation to the training example, and do not use image augmentation with random operations during prediction. Here, we

only use the simplest random left-right flipping method. In addition, we use a `ToTensor` instance to convert mini-batch images into the format required by MXNet, i.e. 32-bit floating point numbers with the shape of (batch size, number of channels, height, width) and value range between 0 and 1.

```
train_augs = gluon.data.vision.transforms.Compose([
    gluon.data.vision.transforms.RandomFlipLeftRight(),
    gluon.data.vision.transforms.ToTensor()])

test_augs = gluon.data.vision.transforms.Compose([
    gluon.data.vision.transforms.ToTensor()])
```

Next, we define an auxiliary function to make it easier to read the image and apply image augmentation. The `transform_first` function provided by Gluon's data set applies image augmentation to the first element of each training example (image and label), i.e., the element at the top of the image. For detailed description of `DataLoader`, refer to [Section 5.5](#).

```
def load_cifar10(is_train, augs, batch_size):
    return gluon.data.DataLoader(
        gluon.data.vision.CIFAR10(train=is_train).transform_first(augs),
        batch_size=batch_size, shuffle=is_train,
        num_workers=d2l.get_dataloader_workers())
```

## Using a Multi-GPU Training Model

We train the ResNet-18 model described in [Section 9.6](#) on the CIFAR-10 data set. We will also apply the methods described in [Section 13.5](#) and use a multi-GPU training model.

Next, we define the training function to train and evaluate the model using multiple GPUs.

```
# Save to the d2l package.
def train_batch_ch12(net, features, labels, loss, trainer, ctx_list):
    Xs, ys = d2l.split_batch(features, labels, ctx_list)
    with autograd.record():
        pys = [net(X) for X in Xs]
        ls = [loss(py, y) for py, y in zip(pys, ys)]
    for l in ls:
        l.backward()
    trainer.step(features.shape[0])
    train_loss_sum = sum([l.sum().asscalar() for l in ls])
    train_acc_sum = sum(d2l.accuracy(py, y) for py, y in zip(pys, ys))
    return train_loss_sum, train_acc_sum
```

```
# Save to the d2l package.
def train_ch12(net, train_iter, test_iter, loss, trainer, num_epochs,
              ctx_list=d2l.try_all_gpus()):
    num_batches, timer = len(train_iter), d2l.Timer()
    animator = d2l.Animator(xlabel='epoch', xlim=[0,num_epochs], ylim=[0,2],
                            legend=['train loss', 'train acc', 'test acc'])
    for epoch in range(num_epochs):
        # store training_loss, training_accuracy, num_examples, num_features
        metric = d2l.Accumulator(4)
        for i, (features, labels) in enumerate(train_iter):
            timer.start()
```

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```

l, acc = train_batch_ch12(
    net, features, labels, loss, trainer, ctx_list)
metric.add(l, acc, labels.shape[0], labels.size)
timer.stop()
if (i+1) % (num_batches // 5) == 0:
    animator.add(epoch+i/num_batches,
                 (metric[0]/metric[2], metric[1]/metric[3], None))
test_acc = d2l.evaluate_accuracy_gpus(net, test_iter)
animator.add(epoch+1, (None, None, test_acc))
print('loss %.3f, train acc %.3f, test acc %.3f' %
      (metric[0]/metric[2], metric[1]/metric[3], test_acc))
print('%.1f examples/sec on %s' %
      (metric[2]*num_epochs/timer.sum(), ctx_list))

```

Now, we can define the `train_with_data_aug` function to use image augmentation to train the model. This function obtains all available GPUs and uses Adam as the optimization algorithm for training. It then applies image augmentation to the training data set, and finally calls the `train` function just defined to train and evaluate the model.

```

def train_with_data_aug(train_augs, test_augs, lr=0.001):
    batch_size, ctx, net = 256, d2l.try_all_gpus(), d2l.resnet18(10)
    net.initialize(ctx=ctx, init=init.Xavier())
    trainer = gluon.Trainer(net.collect_params(), 'adam',
                           {'learning_rate': lr})
    loss = gluon.loss.SoftmaxCrossEntropyLoss()
    train_iter = load_cifar10(True, train_augs, batch_size)
    test_iter = load_cifar10(False, test_augs, batch_size)
    train_ch12(net, train_iter, test_iter, loss, trainer, 10, ctx)

```

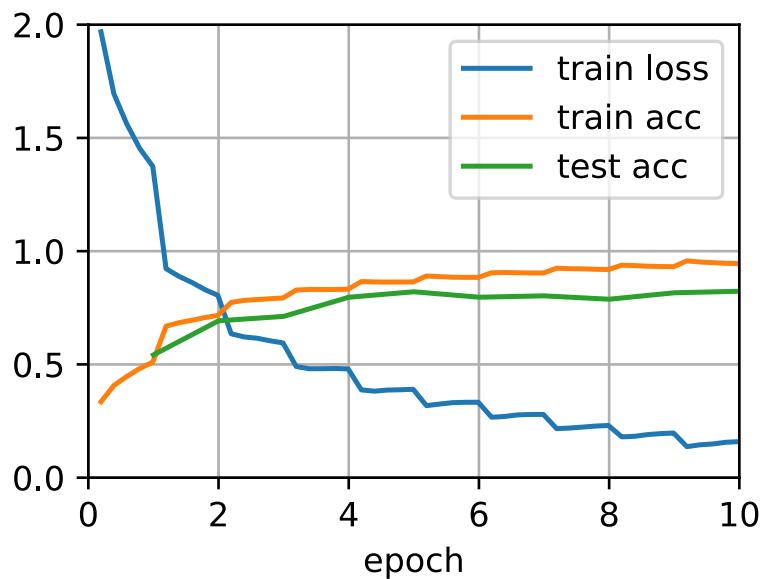
Now we train the model using image augmentation of random flipping left and right.

```
train_with_data_aug(train_augs, test_augs)
```

```

loss 0.159, train acc 0.945, test acc 0.823
5427.3 examples/sec on [gpu(0), gpu(1)]

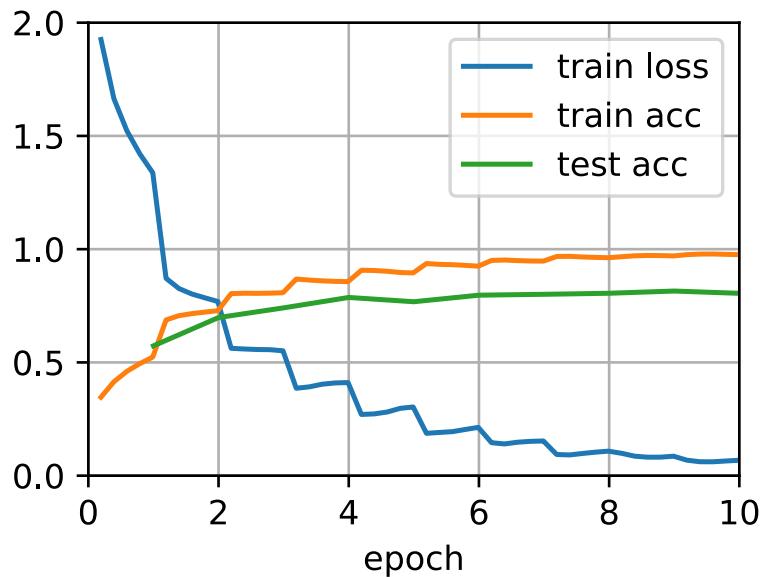
```



Compare to training without image augmentation.

```
train_with_data_aug(test_augs, test_augs)
```

```
loss 0.068, train acc 0.976, test acc 0.805
5472.5 examples/sec on [gpu(0), gpu(1)]
```



### 14.1.3 Summary

- Image augmentation generates random images based on existing training data to cope with overfitting.
- In order to obtain a definitive results during prediction, we usually only apply image augmentation to the training example, and do not use image augmentation with random operations during prediction.

- We can obtain classes related to image augmentation from Gluon's `transforms` module.

#### 14.1.4 Exercises

- Train the model without using image augmentation: `train_with_data_aug(no_aug, no_aug)`. Compare training and testing accuracy when using and not using image augmentation. Can this comparative experiment support the argument that image augmentation can mitigate overfitting? Why?
- Add different image augmentation methods in model training based on the CIFAR-10 data set. Observe the implementation results.
- With reference to the MXNet documentation, what other image augmentation methods are provided in Gluon's `transforms` module?

#### 14.1.5 Scan the QR Code to Discuss<sup>176</sup>



## 14.2 Fine Tuning

In earlier chapters, we discussed how to train models on the Fashion-MNIST training data set, which only has 60,000 images. We also described ImageNet, the most widely used large-scale image data set in the academic world, with more than 10 million images and objects of over 1000 categories. However, the size of data sets that we often deal with is usually larger than the first, but smaller than the second.

Assume we want to identify different kinds of chairs in images and then push the purchase link to the user. One possible method is to first find a hundred common chairs, take one thousand different images with different angles for each chair, and then train a classification model on the collected image data set. Although this data set may be larger than Fashion-MNIST, the number of examples is still less than one tenth of ImageNet. This may result in the overfitting of the complicated model applicable to ImageNet on this data set. At the same time, because of the limited amount of data, the accuracy of the final trained model may not meet the practical requirements.

In order to deal with the above problems, an obvious solution is to collect more data. However, collecting and labeling data can consume a lot of time and money. For example, in order to collect the ImageNet data sets, researchers have spent millions of dollars of research funding. Although, recently, data collection costs have dropped significantly, the costs still cannot be ignored.

Another solution is to apply transfer learning to migrate the knowledge learned from the source data set to the target data set. For example, although the images in ImageNet are mostly unrelated to chairs, models trained on this data set can extract more general image features that can help identify edges, textures, shapes, and object composition. These similar features may be equally effective for recognizing a chair.

In this section, we introduce a common technique in transfer learning: fine tuning. As shown in Figure 11.1, fine tuning consists of the following four steps:

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<sup>176</sup> <https://discuss.mxnet.io/t/2442>

1. Pre-train a neural network model, i.e., the source model, on a source data set (e.g., the ImageNet data set).
2. Create a new neural network model, i.e., the target model. This replicates all model designs and their parameters on the source model, except the output layer. We assume that these model parameters contain the knowledge learned from the source data set and this knowledge will be equally applicable to the target data set. We also assume that the output layer of the source model is closely related to the labels of the source data set and is therefore not used in the target model.
3. Add an output layer whose output size is the number of target data set categories to the target model, and randomly initialize the model parameters of this layer.
4. Train the target model on a target data set, such as a chair data set. We will train the output layer from scratch, while the parameters of all remaining layers are fine tuned based on the parameters of the source model.

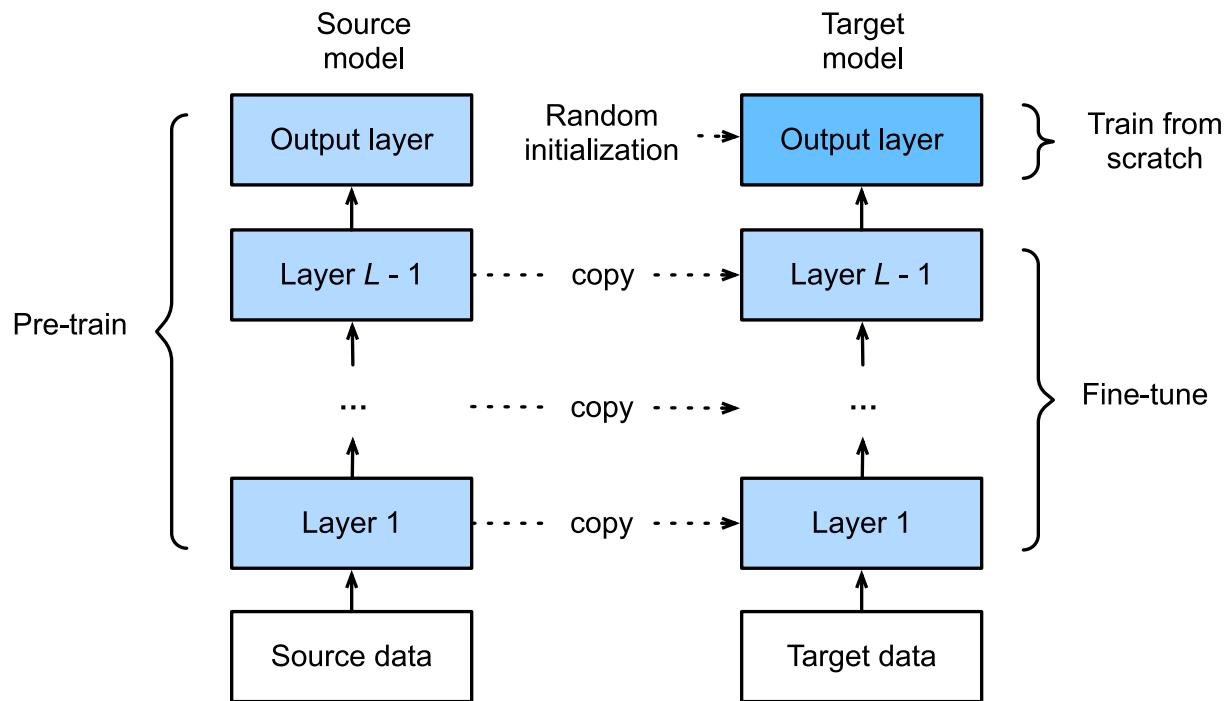


Fig. 14.2.1: Fine tuning.

### 14.2.1 Hot Dog Recognition

Next, we will use a specific example for practice: hot dog recognition. We will fine tune the ResNet model trained on the ImageNet data set based on a small data set. This small data set contains thousands of images, some of which contain hot dogs. We will use the model obtained by fine tuning to identify whether an image contains a hot dog.

First, import the packages and modules required for the experiment. Gluon's `model_zoo` package provides a common pre-trained model. If you want to get more pre-trained models for computer vision, you can use the `GluonCV Toolkit`<sup>177</sup>.

<sup>177</sup> <https://gluon-cv.mxnet.io>

```
%matplotlib inline
import d2l
from mxnet import gluon, init, nd
from mxnet.gluon import nn
import os
import zipfile
```

## Get the Data Set

The hot dog data set we use was taken from online images and contains 1,400 positive images containing hot dogs and same number of negative images containing other foods. 1,000 images of various classes are used for training and the rest are used for testing.

We first download the compressed data set to the path `../data`. Then, we unzip the downloaded data set in this path and get two folders, `hotdog/train` and `hotdog/test`. Both folders have `hotdog` and `not-hotdog` category subfolders, each of which has corresponding image files.

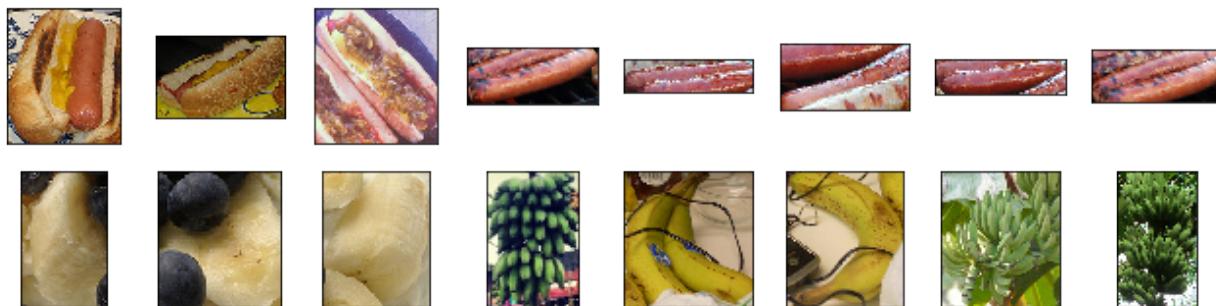
```
data_dir = '../data'
base_url = 'https://apache-mxnet.s3-accelerate.amazonaws.com/'
fname = gluon.utils.download(
    base_url + 'gluon/dataset/hotdog.zip',
    path=data_dir, sha1_hash='fba480ffa8aa7e0feb511d181409f899b9baa5')
with zipfile.ZipFile(fname, 'r') as z:
    z.extractall(data_dir)
```

We create two `ImageFolderDataset` instances to read all the image files in the training data set and testing data set, respectively.

```
train_imgs = gluon.data.vision.ImageFolderDataset(
    os.path.join(data_dir, 'hotdog/train'))
test_imgs = gluon.data.vision.ImageFolderDataset(
    os.path.join(data_dir, 'hotdog/test'))
```

The first 8 positive examples and the last 8 negative images are shown below. As you can see, the images vary in size and aspect ratio.

```
hotdogs = [train_imgs[i][0] for i in range(8)]
not_hotdogs = [train_imgs[-i - 1][0] for i in range(8)]
d2l.show_images(hotdogs + not_hotdogs, 2, 8, scale=1.4);
```



During training, we first crop a random area with random size and random aspect ratio from the image and then scale the area to an input with a height and width of 224 pixels. During testing, we scale the height

and width of images to 256 pixels, and then crop the center area with height and width of 224 pixels to use as the input. In addition, we normalize the values of the three RGB (red, green, and blue) color channels. The average of all values of the channel is subtracted from each value and then the result is divided by the standard deviation of all values of the channel to produce the output.

```
# We specify the mean and variance of the three RGB channels to normalize the image
# channel.
normalize = gluon.data.vision.transforms.Normalize(
    [0.485, 0.456, 0.406], [0.229, 0.224, 0.225])

train_augs = gluon.data.vision.transforms.Compose([
    gluon.data.vision.transforms.RandomResizedCrop(224),
    gluon.data.vision.transforms.RandomFlipLeftRight(),
    gluon.data.vision.transforms.ToTensor(),
    normalize])

test_augs = gluon.data.vision.transforms.Compose([
    gluon.data.vision.transforms.Resize(256),
    gluon.data.vision.transforms.CenterCrop(224),
    gluon.data.vision.transforms.ToTensor(),
    normalize])
```

## Define and Initialize the Model

We use ResNet-18, which was pre-trained on the ImageNet data set, as the source model. Here, we specify `pretrained=True` to automatically download and load the pre-trained model parameters. The first time they are used, the model parameters need to be downloaded from the Internet.

```
pretrained_net = gluon.model_zoo.vision.resnet18_v2(pretrained=True)
```

The pre-trained source model instance contains two member variables: `features` and `output`. The former contains all layers of the model, except the output layer, and the latter is the output layer of the model. The main purpose of this division is to facilitate the fine tuning of the model parameters of all layers except the output layer. The member variable `output` of source model is given below. As a fully connected layer, it transforms ResNet's final global average pooling layer output into 1000 class output on the ImageNet data set.

```
pretrained_net.output
```

```
Dense(512 -> 1000, linear)
```

We then build a new neural network to use as the target model. It is defined in the same way as the pre-trained source model, but the final number of outputs is equal to the number of categories in the target data set. In the code below, the model parameters in the member variable `features` of the target model instance `finetune_net` are initialized to model parameters of the corresponding layer of the source model. Because the model parameters in `features` are obtained by pre-training on the ImageNet data set, it is good enough. Therefore, we generally only need to use small learning rates to “fine tune” these parameters. In contrast, model parameters in the member variable `output` are randomly initialized and generally require a larger learning rate to learn from scratch. Assume the learning rate in the `Trainer` instance is  $\eta$  and use a learning rate of  $10\eta$  to update the model parameters in the member variable `output`.

```
finetune_net = gluon.model_zoo.vision.resnet18_v2(classes=2)
finetune_net.features = pretrained_net.features
```

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```
finetune_net.output.initialize(init.Xavier())
# The model parameters in output will be updated using a learning rate ten
# times greater
finetune_net.output.collect_params().setattr('lr_mult', 10)
```

## Fine Tune the Model

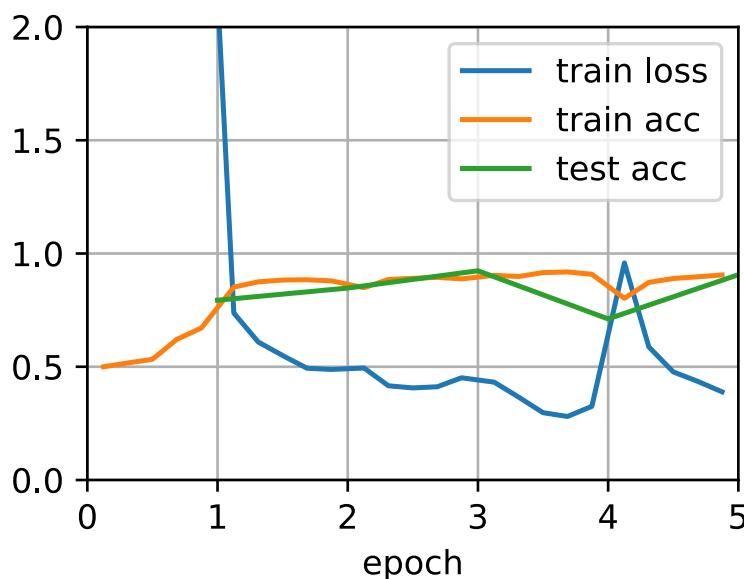
We first define a training function `train_fine_tuning` that uses fine tuning so it can be called multiple times.

```
def train_fine_tuning(net, learning_rate, batch_size=128, num_epochs=5):
    train_iter = gluon.data.DataLoader(
        train_imgs.transform_first(train_augs), batch_size, shuffle=True)
    test_iter = gluon.data.DataLoader(
        test_imgs.transform_first(test_augs), batch_size)
    ctx = d2l.try_all_gpus()
    net.collect_params().reset_ctx(ctx)
    net.hybridize()
    loss = gluon.loss.SoftmaxCrossEntropyLoss()
    trainer = gluon.Trainer(net.collect_params(), 'sgd', {
        'learning_rate': learning_rate, 'wd': 0.001})
    d2l.train_ch12(net, train_iter, test_iter, loss, trainer, num_epochs, ctx)
```

We set the learning rate in the `Trainer` instance to a smaller value, such as 0.01, in order to fine tune the model parameters obtained in pre-training. Based on the previous settings, we will train the output layer parameters of the target model from scratch using a learning rate ten times greater.

```
train_fine_tuning(finetune_net, 0.01)
```

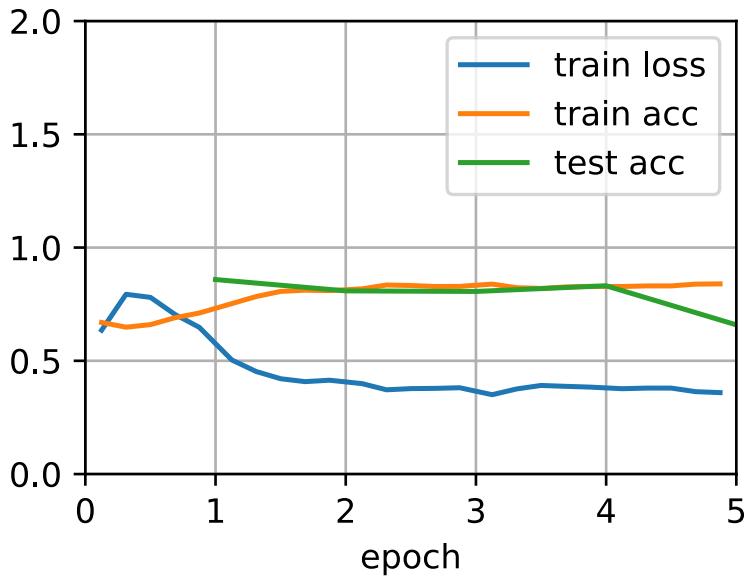
```
loss 0.393, train acc 0.904, test acc 0.906
637.1 examples/sec on [gpu(0), gpu(1)]
```



For comparison, we define an identical model, but initialize all of its model parameters to random values. Since the entire model needs to be trained from scratch, we can use a larger learning rate.

```
scratch_net = gluon.model_zoo.vision.resnet18_v2(classes=2)
scratch_net.initialize(init=init.Xavier())
train_fine_tuning(scratch_net, 0.1)
```

```
loss 0.363, train acc 0.837, test acc 0.659
673.0 examples/sec on [gpu(0), gpu(1)]
```



As you can see, the fine-tuned model tends to achieve higher precision in the same epoch because the initial values of the parameters are better.

### 14.2.2 Summary

- Transfer learning migrates the knowledge learned from the source data set to the target data set. Fine tuning is a common technique for transfer learning.
- The target model replicates all model designs and their parameters on the source model, except the output layer, and fine tunes these parameters based on the target data set. In contrast, the output layer of the target model needs to be trained from scratch.
- Generally, fine tuning parameters use a smaller learning rate, while training the output layer from scratch can use a larger learning rate.

### 14.2.3 Exercises

- Keep increasing the learning rate of `finetune_net`. How does the precision of the model change?
- Further tune the hyper-parameters of `finetune_net` and `scratch_net` in the comparative experiment. Do they still have different precisions?
- Set the parameters in `finetune_net.features` to the parameters of the source model and do not update them during training. What will happen? You can use the following code.

```
finetune_net.features.collect_params().setattr('grad_req', 'null')
```

- In fact, there is also a “hotdog” class in the ImageNet data set. Its corresponding weight parameter at the output layer can be obtained by using the following code. How can we use this parameter?

```
weight = pretrained_net.output.weight
hotdog_w = nd.split(weight.data(), 1000, axis=0)[713]
hotdog_w.shape
```

```
(1, 512)
```

#### 14.2.4 Scan the QR Code to Discuss<sup>178</sup>



### 14.3 Object Detection and Bounding Boxes

In the previous section, we introduced many models for image classification. In image classification tasks, we assume that there is only one main target in the image and we only focus on how to identify the target category. However, in many situations, there are multiple targets in the image that we are interested in. We not only want to classify them, but also want to obtain their specific positions in the image. In computer vision, we refer to such tasks as object detection (or object recognition).

Object detection is widely used in many fields. For example, in self-driving technology, we need to plan routes by identifying the locations of vehicles, pedestrians, roads, and obstacles in the captured video image. Robots often perform this type of task to detect targets of interest. Systems in the security field need to detect abnormal targets, such as intruders or bombs.

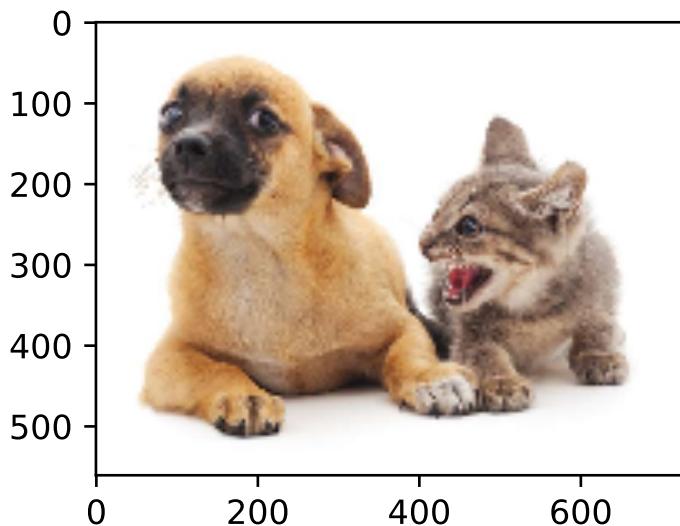
In the next few sections, we will introduce multiple deep learning models used for object detection. Before that, we should discuss the concept of target location. First, import the packages and modules required for the experiment.

```
%matplotlib inline
import d2l
from mxnet import image
```

Next, we will load the sample images that will be used in this section. We can see there is a dog on the left side of the image and a cat on the right. They are the two main targets in this image.

```
d2l.set_figsize((3.5, 2.5))
img = image.imread('../img/catdog.jpg').asnumpy()
d2l.plt.imshow(img);
```

<sup>178</sup> <https://discuss.mxnet.io/t/2443>



### 14.3.1 Bounding Box

In object detection, we usually use a bounding box to describe the target location. The bounding box is a rectangular box that can be determined by the  $x$  and  $y$  axis coordinates in the upper-left corner and the  $x$  and  $y$  axis coordinates in the lower-right corner of the rectangle. We will define the bounding boxes of the dog and the cat in the image based on the coordinate information in the above image. The origin of the coordinates in the above image is the upper left corner of the image, and to the right and down are the positive directions of the  $x$  axis and the  $y$  axis, respectively.

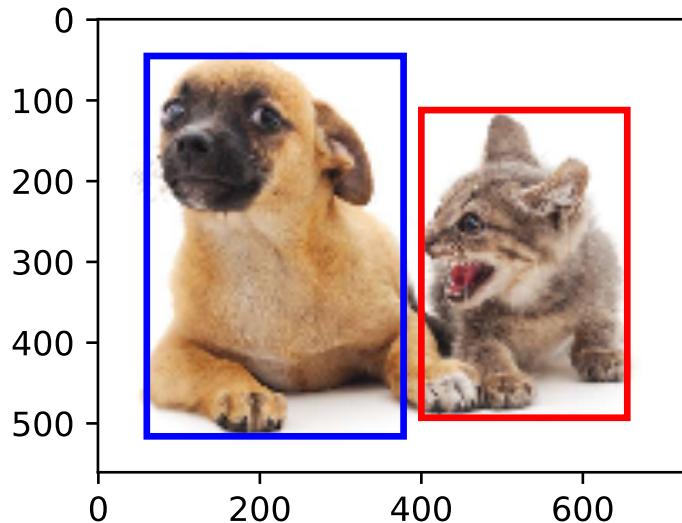
```
# bbox is the abbreviation for bounding box
dog_bbox, cat_bbox = [60, 45, 378, 516], [400, 112, 655, 493]
```

We can draw the bounding box in the image to check if it is accurate. Before drawing the box, we will define a helper function `bbox_to_rect`. It represents the bounding box in the bounding box format of matplotlib.

```
# Save to the d2l package.
def bbox_to_rect(bbox, color):
    """Convert bounding box to matplotlib format."""
    # Convert the bounding box (top-left x, top-left y, bottom-right x,
    # bottom-right y) format to matplotlib format: ((upper-left x,
    # upper-left y), width, height)
    return d2l.plt.Rectangle(
        xy=(bbox[0], bbox[1]), width=bbox[2]-bbox[0], height=bbox[3]-bbox[1],
        fill=False, edgecolor=color, linewidth=2)
```

After loading the bounding box on the image, we can see that the main outline of the target is basically inside the box.

```
fig = d2l.plt.imshow(img)
fig.axes.add_patch(bbox_to_rect(dog_bbox, 'blue'))
fig.axes.add_patch(bbox_to_rect(cat_bbox, 'red'));
```



### 14.3.2 Summary

- In object detection, we not only need to identify all the objects of interest in the image, but also their positions. The positions are generally represented by a rectangular bounding box.

### 14.3.3 Exercises

- Find some images and try to label a bounding box that contains the target. Compare the difference between the time it takes to label the bounding box and label the category.

### 14.3.4 Scan the QR Code to Discuss<sup>179</sup>



## 14.4 Anchor Boxes

Object detection algorithms usually sample a large number of regions in the input image, determine whether these regions contain objects of interest, and adjust the edges of the regions so as to predict the ground-truth bounding box of the target more accurately. Different models may use different region sampling methods. Here, we introduce one such method: it generates multiple bounding boxes with different sizes and aspect ratios while centering on each pixel. These bounding boxes are called anchor boxes. We will practice object detection based on anchor boxes in the following sections.

---

<sup>179</sup> <https://discuss.mxnet.io/t/2444>

First, import the packages or modules required for this section. Here, we have introduced the `contrib` package, and modified the printing accuracy of NumPy. Because printing NDArray actually calls the print function of NumPy, the floating-point numbers in NDArray printed in this section are more concise.

```
%matplotlib inline
import d2l
from mxnet import contrib, gluon, image, nd
import numpy as np
np.set_printoptions(2)
```

#### 14.4.1 Generate Multiple Anchor Boxes

Assume the input image has a height of  $h$  and width of  $w$ . We generate anchor boxes with different shapes centered on each pixel of the image. Assume the size is  $s \in (0, 1]$ , the aspect ratio is  $r > 0$ , and the width and height of the anchor box are  $ws\sqrt{r}$  and  $hs/\sqrt{r}$ , respectively. When the center position is given, an anchor box with known width and height is determined.

Below we set a set of sizes  $s_1, \dots, s_n$  and a set of aspect ratios  $r_1, \dots, r_m$ . If we use a combination of all sizes and aspect ratios with each pixel as the center, the input image will have a total of  $whnm$  anchor boxes. Although these anchor boxes may cover all ground-truth bounding boxes, the computational complexity is often excessive. Therefore, we are usually only interested in a combination containing  $s_1$  or  $r_1$  sizes and aspect ratios, that is:

$$(s_1, r_1), (s_1, r_2), \dots, (s_1, r_m), (s_2, r_1), (s_3, r_1), \dots, (s_n, r_1). \quad (14.4.1)$$

That is, the number of anchor boxes centered on the same pixel is  $n + m - 1$ . For the entire input image, we will generate a total of  $wh(n + m - 1)$  anchor boxes.

The above method of generating anchor boxes has been implemented in the `MultiBoxPrior` function. We specify the input, a set of sizes, and a set of aspect ratios, and this function will return all the anchor boxes entered.

```
img = image.imread('../img/catdog.jpg').asnumpy()
h, w = img.shape[0:2]

print(h, w)
X = nd.random.uniform(shape=(1, 3, h, w)) # Construct input data
Y = contrib.nd.MultiBoxPrior(X, sizes=[0.75, 0.5, 0.25], ratios=[1, 2, 0.5])
Y.shape
```

561 728

(1, 2042040, 4)

We can see that the shape of the returned anchor box variable `y` is (batch size, number of anchor boxes, 4). After changing the shape of the anchor box variable `y` to (image height, image width, number of anchor boxes centered on the same pixel, 4), we can obtain all the anchor boxes centered on a specified pixel position. In the following example, we access the first anchor box centered on (250, 250). It has four elements: the  $x, y$  axis coordinates in the upper-left corner and the  $x, y$  axis coordinates in the lower-right corner of the anchor box. The coordinate values of the  $x$  and  $y$  axis are divided by the width and height of the image, respectively, so the value range is between 0 and 1.

```
boxes = Y.reshape((h, w, 5, 4))
boxes[250, 250, 0, :]
```

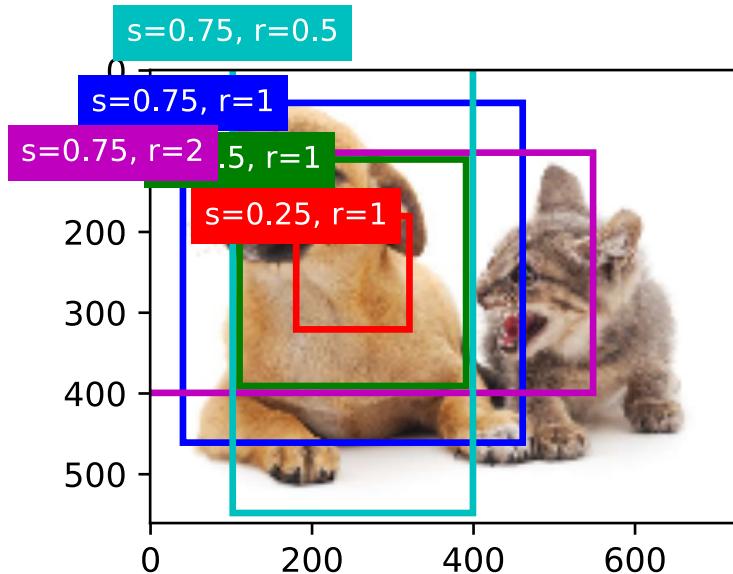
```
[0.06 0.07 0.63 0.82]
<NDArray 4 @cpu(0)>
```

In order to describe all anchor boxes centered on one pixel in the image, we first define the `show_bboxes` function to draw multiple bounding boxes on the image.

```
# Save to the d2l package.
def show_bboxes(axes, bboxes, labels=None, colors=None):
    """Show bounding boxes."""
    def _make_list(obj, default_values=None):
        if obj is None:
            obj = default_values
        elif not isinstance(obj, (list, tuple)):
            obj = [obj]
        return obj
    labels = _make_list(labels)
    colors = _make_list(colors, ['b', 'g', 'r', 'm', 'c'])
    for i, bbox in enumerate(bboxes):
        color = colors[i % len(colors)]
        rect = d2l.bbox_to_rect(bbox.asnumpy(), color)
        axes.add_patch(rect)
        if labels and len(labels) > i:
            text_color = 'k' if color == 'w' else 'w'
            axes.text(rect.xy[0], rect.xy[1], labels[i],
                      va='center', ha='center', fontsize=9, color=text_color,
                      bbox=dict(facecolor=color, lw=0))
```

As we just saw, the coordinate values of the  $x$  and  $y$  axis in the variable `bboxes` have been divided by the width and height of the image, respectively. When drawing images, we need to restore the original coordinate values of the anchor boxes and therefore define the variable `bbox_scale`. Now, we can draw all the anchor boxes centered on (250, 250) in the image. As you can see, the blue anchor box with a size of 0.75 and an aspect ratio of 1 covers the dog in the image well.

```
d2l.set_figsize((3.5, 2.5))
bbox_scale = nd.array((w, h, w, h))
fig = d2l.plt.imshow(img)
show_bboxes(fig.axes, boxes[250, 250, :, :] * bbox_scale,
            ['s=0.75, r=1', 's=0.5, r=1', 's=0.25, r=1', 's=0.75, r=2',
             's=0.75, r=0.5'])
```



#### 14.4.2 Intersection over Union

We just mentioned that the anchor box covers the dog in the image well. If the ground-truth bounding box of the target is known, how can “well” here be quantified? An intuitive method is to measure the similarity between anchor boxes and the ground-truth bounding box. We know that the Jaccard index can measure the similarity between two sets. Given sets  $\mathcal{A}$  and  $\mathcal{B}$ , their Jaccard index is the size of their intersection divided by the size of their union:

$$J(\mathcal{A}, \mathcal{B}) = \frac{|\mathcal{A} \cap \mathcal{B}|}{|\mathcal{A} \cup \mathcal{B}|}. \quad (14.4.2)$$

In fact, we can consider the pixel area of a bounding box as a collection of pixels. In this way, we can measure the similarity of the two bounding boxes by the Jaccard index of their pixel sets. When we measure the similarity of two bounding boxes, we usually refer the Jaccard index as intersection over union (IoU), which is the ratio of the intersecting area to the union area of the two bounding boxes, as shown in Figure 11.2. The value range of IoU is between 0 and 1: 0 means that there are no overlapping pixels between the two bounding boxes, while 1 indicates that the two bounding boxes are equal.

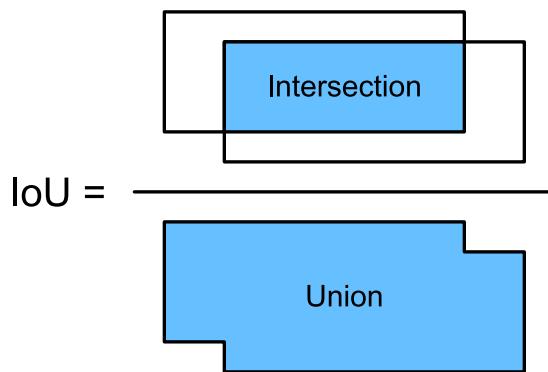


Fig. 14.4.1: IoU is the ratio of the intersecting area to the union area of two bounding boxes.

For the remainder of this section, we will use IoU to measure the similarity between anchor boxes and ground-truth bounding boxes, and between different anchor boxes.

### 14.4.3 Labeling Training Set Anchor Boxes

In the training set, we consider each anchor box as a training example. In order to train the object detection model, we need to mark two types of labels for each anchor box: first, the category of the target contained in the anchor box (category) and, second, the offset of the ground-truth bounding box relative to the anchor box (offset). In object detection, we first generate multiple anchor boxes, predict the categories and offsets for each anchor box, adjust the anchor box position according to the predicted offset to obtain the bounding boxes to be used for prediction, and finally filter out the prediction bounding boxes that need to be output.

We know that, in the object detection training set, each image is labelled with the location of the ground-truth bounding box and the category of the target contained. After the anchor boxes are generated, we primarily label anchor boxes based on the location and category information of the ground-truth bounding boxes similar to the anchor boxes. So how do we assign ground-truth bounding boxes to anchor boxes similar to them?

Assume the anchor boxes in the image are  $A_1, A_2, \dots, A_{n_a}$  and the ground-truth bounding boxes are  $B_1, B_2, \dots, B_{n_b}$  and  $n_a \geq n_b$ . Define matrix  $\mathbf{X} \in \mathbb{R}^{n_a \times n_b}$ , where element  $x_{ij}$  in the  $i$ th row and  $j$ th column is the IoU of the anchor box  $A_i$  to the ground-truth bounding box  $B_j$ . First, we find the largest element in the matrix  $\mathbf{X}$  and record the row index and column index of the element as  $i_1, j_1$ . We assign the ground-truth bounding box  $B_{j_1}$  to the anchor box  $A_{i_1}$ . Obviously, anchor box  $A_{i_1}$  and ground-truth bounding box  $B_{j_1}$  have the highest similarity among all the “anchor box - ground-truth bounding box” pairings. Next, discard all elements in the  $i_1$ th row and the  $j_1$ th column in the matrix  $\mathbf{X}$ . Find the largest remaining element in the matrix  $\mathbf{X}$  and record the row index and column index of the element as  $i_2, j_2$ . We assign ground-truth bounding box  $B_{j_2}$  to anchor box  $A_{i_2}$  and then discard all elements in the  $i_2$ th row and the  $j_2$ th column in the matrix  $\mathbf{X}$ . At this point, elements in two rows and two columns in the matrix  $\mathbf{X}$  have been discarded. We proceed until all elements in the  $n_b$  column in the matrix  $\mathbf{X}$  are discarded. At this time, we have assigned a ground-truth bounding box to each of the  $n_b$  anchor boxes. Next, we only traverse the remaining  $n_a - n_b$  anchor boxes. Given anchor box  $A_i$ , find the bounding box  $B_j$  with the largest IoU with  $A_i$  according to the  $i$ th row of the matrix  $\mathbf{X}$ , and only assign ground-truth bounding box  $B_j$  to anchor box  $A_i$  when the IoU is greater than the predetermined threshold.

As shown in Figure 11.3 (left), assuming that the maximum value in the matrix  $\mathbf{X}$  is  $x_{23}$ , we will assign ground-truth bounding box  $B_3$  to anchor box  $A_2$ . Then, we discard all the elements in row 2 and column 3 of the matrix, find the largest element  $x_{71}$  of the remaining shaded area, and assign ground-truth bounding box  $B_1$  to anchor box  $A_7$ . Then, as shown in Figure 11.3 (middle), discard all the elements in row 7 and column 1 of the matrix, find the largest element  $x_{54}$  of the remaining shaded area, and assign ground-truth bounding box  $B_4$  to anchor box  $A_5$ . Finally, as shown in Figure 11.3 (right), discard all the elements in row 5 and column 4 of the matrix, find the largest element  $x_{92}$  of the remaining shaded area, and assign ground-truth bounding box  $B_2$  to anchor box  $A_9$ . After that, we only need to traverse the remaining anchor boxes of  $A_2, A_5, A_7, A_9$  and determine whether to assign ground-truth bounding boxes to the remaining anchor boxes according to the threshold.

Now we can label the categories and offsets of the anchor boxes. If an anchor box  $A$  is assigned ground-truth bounding box  $B$ , the category of the anchor box  $A$  is set to the category of  $B$  and the offset of the anchor box  $A$  is set according to the relative position of the central coordinates of  $B$  and  $A$  and the relative sizes of the two boxes. Because the positions and sizes of various boxes in the data set may vary, these relative positions and relative sizes usually require some special transformations to make the offset distribution more uniform and easier to fit. Assume the center coordinates of anchor box  $A$  and its assigned ground-truth bounding box  $B$  are  $(x_a, y_a), (x_b, y_b)$ , the widths of  $A$  and  $B$  are  $w_a, w_b$ , and their heights are  $h_a, h_b$ , respectively. In this case, a common technique is to label the offset of  $A$  as

$$\left( \frac{\frac{x_b - x_a}{w_a} - \mu_x}{\sigma_x}, \frac{\frac{y_b - y_a}{h_a} - \mu_y}{\sigma_y}, \frac{\log \frac{w_b}{w_a} - \mu_w}{\sigma_w}, \frac{\log \frac{h_b}{h_a} - \mu_h}{\sigma_h} \right), \quad (14.4.3)$$

The default values of the constant are  $\mu_x = \mu_y = \mu_w = \mu_h = 0, \sigma_x = \sigma_y = 0.1, \text{and } \sigma_w = \sigma_h = 0.2$ . If an anchor box is not assigned a ground-truth bounding box, we only need to set the category of the anchor box

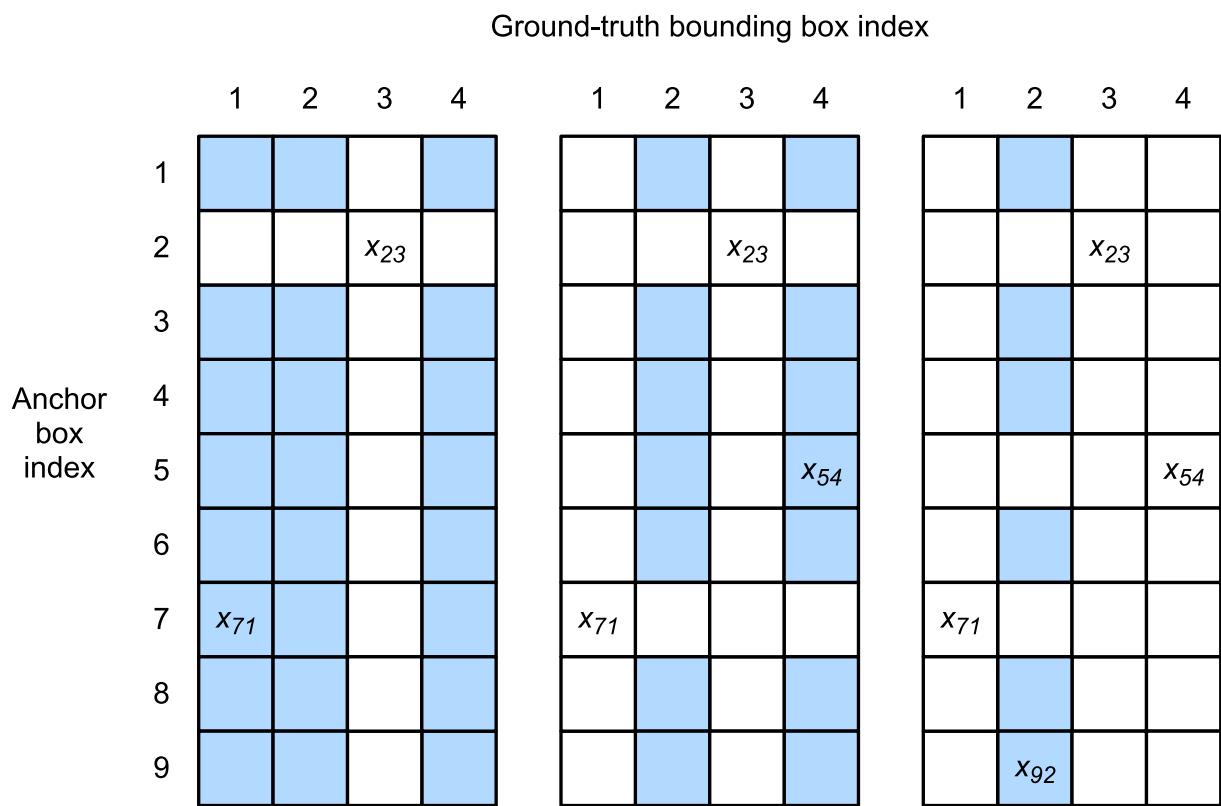
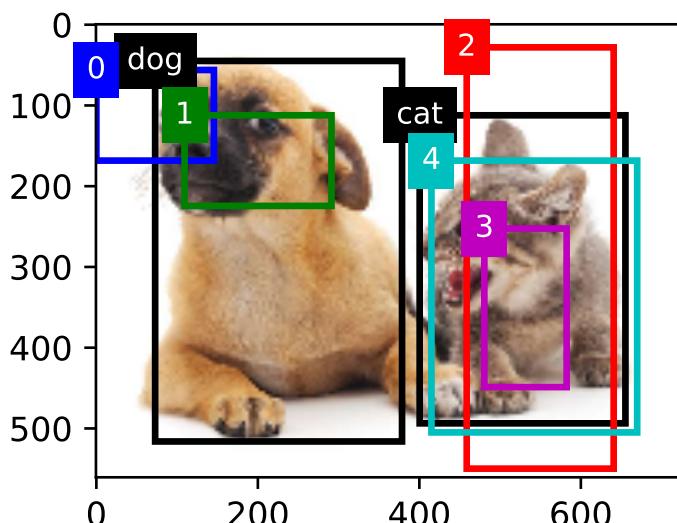


Fig. 14.4.2: Assign ground-truth bounding boxes to anchor boxes.

to background. Anchor boxes whose category is background are often referred to as negative anchor boxes, and the rest are referred to as positive anchor boxes.

Below we demonstrate a detailed example. We define ground-truth bounding boxes for the cat and dog in the read image, where the first element is category (0 for dog, 1 for cat) and the remaining four elements are the  $x, y$  axis coordinates at top-left corner and  $x, y$  axis coordinates at lower-right corner (the value range is between 0 and 1). Here, we construct five anchor boxes to be labeled by the coordinates of the upper-left corner and the lower-right corner, which are recorded as  $A_0, \dots, A_4$ , respectively (the index in the program starts from 0). First, draw the positions of these anchor boxes and the ground-truth bounding boxes in the image.

```
ground_truth = nd.array([[0, 0.1, 0.08, 0.52, 0.92],
                        [1, 0.55, 0.2, 0.9, 0.88]])
anchors = nd.array([[0, 0.1, 0.2, 0.3], [0.15, 0.2, 0.4, 0.4],
                    [0.63, 0.05, 0.88, 0.98], [0.66, 0.45, 0.8, 0.8],
                    [0.57, 0.3, 0.92, 0.9]])
fig = d2l.plt.imshow(img)
show_bboxes(fig.axes, ground_truth[:, 1:] * bbox_scale, ['dog', 'cat'], 'k')
show_bboxes(fig.axes, anchors * bbox_scale, ['0', '1', '2', '3', '4']);
```



We can label categories and offsets for anchor boxes by using the `MultiBoxTarget` function in the `contrib.nd` module. This function sets the background category to 0 and increments the integer index of the target category from zero by 1 (1 for dog and 2 for cat). We add example dimensions to the anchor boxes and ground-truth bounding boxes and construct random predicted results with a shape of (batch size, number of categories including background, number of anchor boxes) by using the `expand_dims` function.

```
labels = contrib.nd.MultiBoxTarget(anchors.expand_dims(axis=0),
                                    ground_truth.expand_dims(axis=0),
                                    nd.zeros((1, 3, 5)))
```

There are three items in the returned result, all of which are in NDArray format. The third item is represented by the category labelled for the anchor box.

```
labels[2]
```

```
[[0. 1. 2. 0. 2.]]  
<NDArray 1x5 @cpu(0)>
```

We analyze these labelled categories based on positions of anchor boxes and ground-truth bounding boxes in the image. First, in all “anchor box - ground-truth bounding box” pairs, the IoU of anchor box  $A_4$  to the ground-truth bounding box of the cat is the largest, so the category of anchor box  $A_4$  is labeled as cat. Without considering anchor box  $A_4$  or the ground-truth bounding box of the cat, in the remaining “anchor box - ground-truth bounding box” pairs, the pair with the largest IoU is anchor box  $A_1$  and the ground-truth bounding box of the dog, so the category of anchor box  $A_1$  is labeled as dog. Next, traverse the remaining three unlabeled anchor boxes. The category of the ground-truth bounding box with the largest IoU with anchor box  $A_0$  is dog, but the IoU is smaller than the threshold (the default is 0.5), so the category is labeled as background; the category of the ground-truth bounding box with the largest IoU with anchor box  $A_2$  is cat and the IoU is greater than the threshold, so the category is labeled as cat; the category of the ground-truth bounding box with the largest IoU with anchor box  $A_3$  is cat, but the IoU is smaller than the threshold, so the category is labeled as background.

The second item of the return value is a mask variable, with the shape of (batch size, four times the number of anchor boxes). The elements in the mask variable correspond one-to-one with the four offset values of each anchor box. Because we don't care about background detection, offsets of the negative class should not affect the target function. By multiplying by element, the 0 in the mask variable can filter out negative class offsets before calculating target function.

labels[1]

```
[[0. 0. 0. 0. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 0. 0. 0. 0. 1. 1. 1. 1. 1.]]  
<NDArray 1x20 @cpu(0)>
```

The first item returned is the four offset values labeled for each anchor box, with the offsets of negative class anchor boxes labeled as 0.

labels[0]

```
[[ 0.00e+00  0.00e+00  0.00e+00  0.00e+00  1.40e+00  1.00e+01  2.59e+00
    7.18e+00 -1.20e+00  2.69e-01  1.68e+00 -1.57e+00  0.00e+00  0.00e+00
    0.00e+00  0.00e+00 -5.71e-01 -1.00e+00 -8.94e-07  6.26e-01]]
<NDArray 1x20 @cpu(0)>
```

#### 14.4.4 Output Bounding Boxes for Prediction

During model prediction phase, we first generate multiple anchor boxes for the image and then predict categories and offsets for these anchor boxes one by one. Then, we obtain prediction bounding boxes based on anchor boxes and their predicted offsets. When there are many anchor boxes, many similar prediction bounding boxes may be output for the same target. To simplify the results, we can remove similar prediction bounding boxes. A commonly used method is called non-maximum suppression (NMS).

Let us take a look at how NMS works. For a prediction bounding box  $B$ , the model calculates the predicted probability for each category. Assume the largest predicted probability is  $p$ , the category corresponding to this probability is the predicted category of  $B$ . We also refer to  $p$  as the confidence level of prediction bounding box  $B$ . On the same image, we sort the prediction bounding boxes with predicted categories other than background by confidence level from high to low, and obtain the list  $L$ . Select the prediction bounding box  $B_1$  with highest confidence level from  $L$  as a baseline and remove all non-benchmark prediction bounding boxes with an IoU with  $B_1$  greater than a certain threshold from  $L$ . The threshold here is a preset hyper-parameter. At this point,  $L$  retains the prediction bounding box with the highest confidence level and

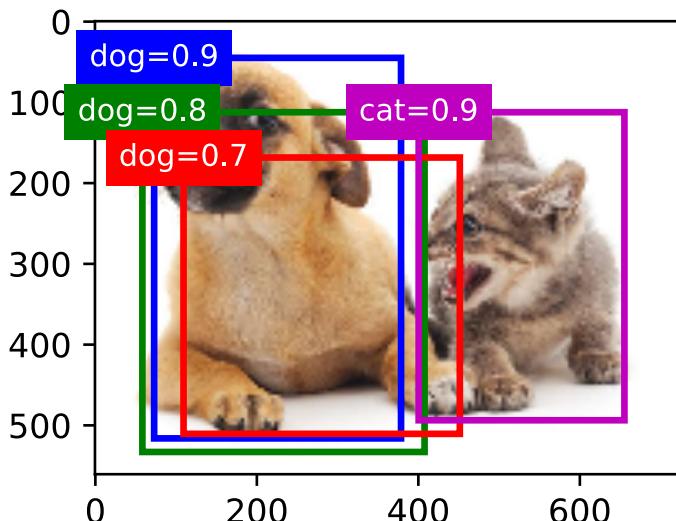
removes other prediction bounding boxes similar to it. Next, select the prediction bounding box  $B_2$  with the second highest confidence level from  $L$  as a baseline, and remove all non-benchmark prediction bounding boxes with an IoU with  $B_2$  greater than a certain threshold from  $L$ . Repeat this process until all prediction bounding boxes in  $L$  have been used as a baseline. At this time, the IoU of any pair of prediction bounding boxes in  $L$  is less than the threshold. Finally, output all prediction bounding boxes in the list  $L$ .

Next, we will look at a detailed example. First, construct four anchor boxes. For the sake of simplicity, we assume that predicted offsets are all 0. This means that the prediction bounding boxes are anchor boxes. Finally, we construct a predicted probability for each category.

```
anchors = nd.array([[0.1, 0.08, 0.52, 0.92], [0.08, 0.2, 0.56, 0.95],
                   [0.15, 0.3, 0.62, 0.91], [0.55, 0.2, 0.9, 0.88]])
offset_preds = nd.array([0] * anchors.size)
cls_probs = nd.array([[0] * 4, # Predicted probability for background
                     [0.9, 0.8, 0.7, 0.1], # Predicted probability for dog
                     [0.1, 0.2, 0.3, 0.9]]) # Predicted probability for cat
```

Print prediction bounding boxes and their confidence levels on the image.

```
fig = d2l.plt.imshow(img)
show_bboxes(fig.axes, anchors * bbox_scale,
            ['dog=0.9', 'dog=0.8', 'dog=0.7', 'cat=0.9'])
```



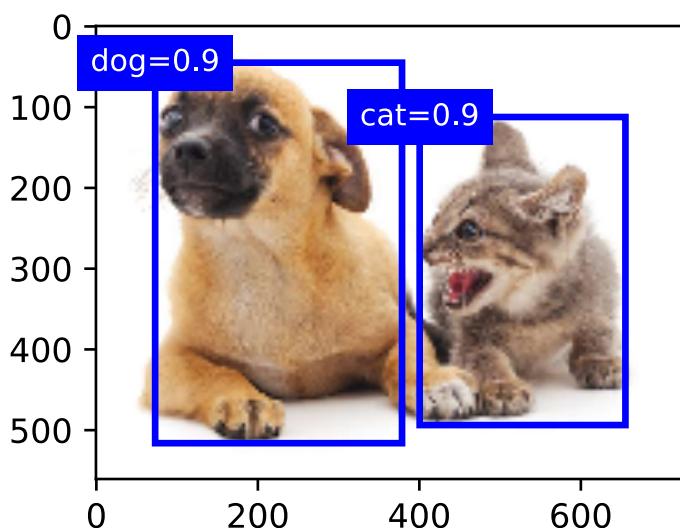
We use the `MultiBoxDetection` function of the `contrib.ndarray` module to perform NMS and set the threshold to 0.5. This adds an example dimension to the NDArray input. We can see that the shape of the returned result is (batch size, number of anchor boxes, 6). The 6 elements of each row represent the output information for the same prediction bounding box. The first element is the predicted category index, which starts from 0 (0 is dog, 1 is cat). The value -1 indicates background or removal in NMS. The second element is the confidence level of prediction bounding box. The remaining four elements are the  $x, y$  axis coordinates of the upper-left corner and the  $x, y$  axis coordinates of the lower-right corner of the prediction bounding box (the value range is between 0 and 1).

```
output = contrib.ndarray.MultiBoxDetection(
    cls_probs.expand_dims(axis=0), offset_preds.expand_dims(axis=0),
    anchors.expand_dims(axis=0), nms_threshold=0.5)
output
```

```
[[[ 0.      0.9     0.1     0.08   0.52    0.92]
 [ 1.      0.9     0.55    0.2     0.9     0.88]
 [-1.     0.8     0.08    0.2     0.56    0.95]
 [-1.     0.7     0.15    0.3     0.62    0.91]]]
<NDArray 1x4x6 @cpu(0)>
```

We remove the prediction bounding boxes of category -1 and visualize the results retained by NMS.

```
fig = d2l.plt.imshow(img)
for i in output[0].asnumpy():
    if i[0] == -1:
        continue
    label = ('dog=' + str(i[0])) + 'cat=' + str(i[1])
    show_bboxes(fig.axes, [nd.array(i[2:]) * bbox_scale], label)
```



In practice, we can remove prediction bounding boxes with lower confidence levels before performing NMS, thereby reducing the amount of computation for NMS. We can also filter the output of NMS, for example, by only retaining results with higher confidence levels as the final output.

#### 14.4.5 Summary

- We generate multiple anchor boxes with different sizes and aspect ratios, centered on each pixel.
- IoU, also called Jaccard index, measures the similarity of two bounding boxes. It is the ratio of the intersecting area to the union area of two bounding boxes.
- In the training set, we mark two types of labels for each anchor box: one is the category of the target contained in the anchor box and the other is the offset of the ground-truth bounding box relative to the anchor box.
- When predicting, we can use non-maximum suppression (NMS) to remove similar prediction bounding boxes, thereby simplifying the results.

### 14.4.6 Exercises

- Change the `sizes` and `ratios` values in `contrib.nd.MultiBoxPrior` and observe the changes to the generated anchor boxes.
- Construct two bounding boxes with an IoU of 0.5, and observe their coincidence.
- Verify the output of offset `labels[0]` by marking the anchor box offsets as defined in this section (the constant is the default value).
- Modify the variable `anchors` in the “Labeling Training Set Anchor Boxes” and “Output Bounding Boxes for Prediction” sections. How do the results change?

### 14.4.7 Scan the QR Code to Discuss<sup>180</sup>



## 14.5 Multiscale Object Detection

In Section 14.4, we generated multiple anchor boxes centered on each pixel of the input image. These anchor boxes are used to sample different regions of the input image. However, if anchor boxes are generated centered on each pixel of the image, soon there will be too many anchor boxes for us to compute. For example, we assume that the input image has a height and a width of 561 and 728 pixels respectively. If five different shapes of anchor boxes are generated centered on each pixel, over two million anchor boxes ( $561 \times 728 \times 5$ ) need to be predicted and labeled on the image.

It is not difficult to reduce the number of anchor boxes. An easy way is to apply uniform sampling on a small portion of pixels from the input image and generate anchor boxes centered on the sampled pixels. In addition, we can generate anchor boxes of varied numbers and sizes on multiple scales. Notice that smaller objects are more likely to be positioned on the image than larger ones. Here, we will use a simple example: Objects with shapes of  $1 \times 1$ ,  $1 \times 2$ , and  $2 \times 2$  may have 4, 2, and 1 possible position(s) on an image with the shape  $2 \times 2$ . Therefore, when using smaller anchor boxes to detect smaller objects, we can sample more regions; when using larger anchor boxes to detect larger objects, we can sample fewer regions.

To demonstrate how to generate anchor boxes on multiple scales, let us read an image first. It has a height and width of  $561 * 728$  pixels.

```
%matplotlib inline
import d2l
from mxnet import contrib, image, nd

img = image.imread('../img/catdog.jpg')
h, w = img.shape[0:2]
h, w
```

---

<sup>180</sup> <https://discuss.mxnet.io/t/2445>

(561, 728)

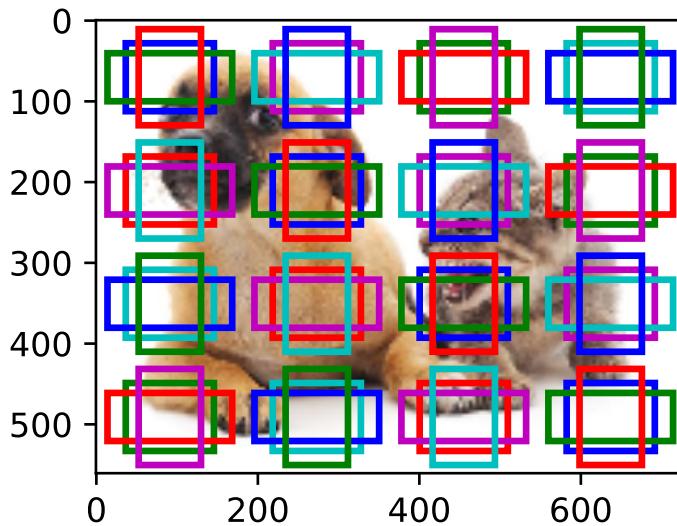
In Section 8.2, the 2D array output of the convolutional neural network (CNN) is called a feature map. We can determine the midpoints of anchor boxes uniformly sampled on any image by defining the shape of the feature map.

The function `display_anchors` is defined below. We are going to generate anchor boxes `anchors` centered on each unit (pixel) on the feature map `fmap`. Since the coordinates of axes  $x$  and  $y$  in anchor boxes `anchors` have been divided by the width and height of the feature map `fmap`, values between 0 and 1 can be used to represent relative positions of anchor boxes in the feature map. Since the midpoints of anchor boxes `anchors` overlap with all the units on feature map `fmap`, the relative spatial positions of the midpoints of the `anchors` on any image must have a uniform distribution. Specifically, when the width and height of the feature map are set to `fmap_w` and `fmap_h` respectively, the function will conduct uniform sampling for `fmap_h` rows and `fmap_w` columns of pixels and use them as midpoints to generate anchor boxes with size `s` (we assume that the length of list `s` is 1) and different aspect ratios (`ratios`).

```
def display_anchors(fmap_w, fmap_h, s):
    d2l.set_figsize((3.5, 2.5))
    # The values from the first two dimensions will not affect the output
    fmap = nd.zeros((1, 10, fmap_w, fmap_h))
    anchors = contrib.nd.MultiBoxPrior(fmap, sizes=s, ratios=[1, 2, 0.5])
    bbox_scale = nd.array((w, h, w, h))
    d2l.show_bboxes(d2l.plt.imshow(img.asnumpy()).axes,
                    anchors[0] * bbox_scale)
```

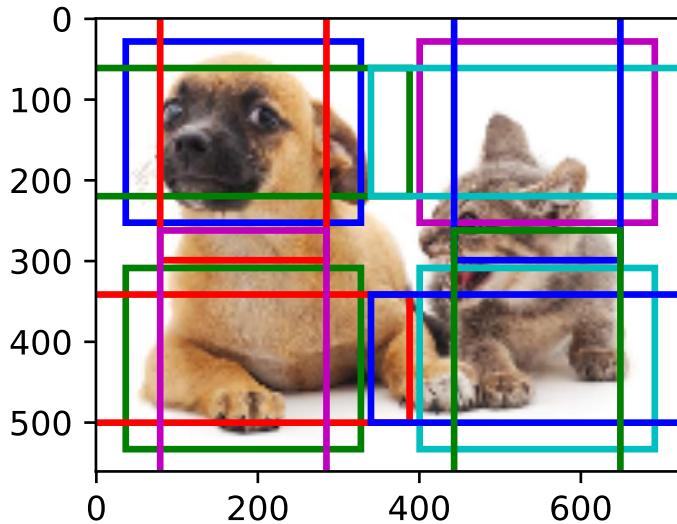
We will first focus on the detection of small objects. In order to make it easier to distinguish upon display, the anchor boxes with different midpoints here do not overlap. We assume that the size of the anchor boxes is 0.15 and the height and width of the feature map are 4. We can see that the midpoints of anchor boxes from the 4 rows and 4 columns on the image are uniformly distributed.

```
display_anchors(fmap_w=4, fmap_h=4, s=[0.15])
```



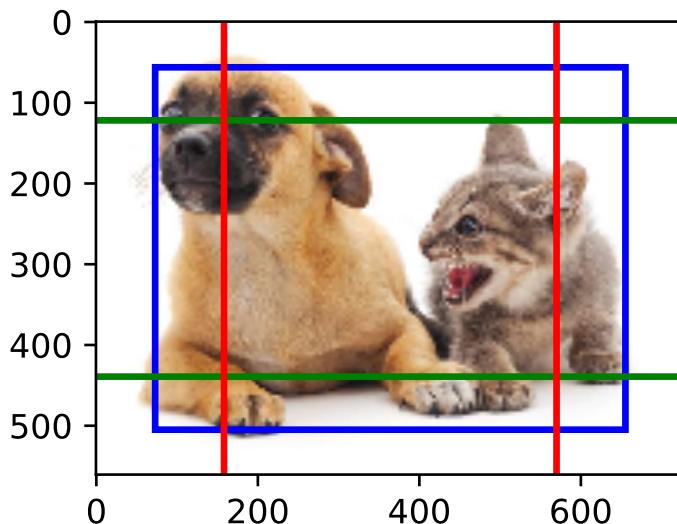
We are going to reduce the height and width of the feature map by half and use a larger anchor box to detect larger objects. When the size is set to 0.4, overlaps will occur between regions of some anchor boxes.

```
display_anchors(fmap_w=2, fmap_h=2, s=[0.4])
```



Finally, we are going to reduce the height and width of the feature map by half and increase the anchor box size to 0.8. Now the midpoint of the anchor box is the center of the image.

```
display_anchors(fmap_w=1, fmap_h=1, s=[0.8])
```



Since we have generated anchor boxes of different sizes on multiple scales, we will use them to detect objects of various sizes at different scales. Now we are going to introduce a method based on convolutional neural networks (CNNs).

At a certain scale, suppose we generate  $h \times w$  sets of anchor boxes with different midpoints based on  $c_i$  feature maps with the shape  $h \times w$  and the number of anchor boxes in each set is  $a$ . For example, for the first scale of the experiment, we generate 16 sets of anchor boxes with different midpoints based on 10 (number of channels) feature maps with a shape of  $4 \times 4$ , and each set contains 3 anchor boxes. Next, each anchor box is labeled with a category and offset based on the classification and position of the ground-truth bounding box. At the current scale, the object detection model needs to predict the category and offset of

$h \times w$  sets of anchor boxes with different midpoints based on the input image.

We assume that the  $c_i$  feature maps are the intermediate output of the CNN based on the input image. Since each feature map has  $h \times w$  different spatial positions, the same position will have  $c_i$  units. According to the definition of receptive field in the [Section 8.2](#), the  $c_i$  units of the feature map at the same spatial position have the same receptive field on the input image. Thus, they represent the information of the input image in this same receptive field. Therefore, we can transform the  $c_i$  units of the feature map at the same spatial position into the categories and offsets of the  $a$  anchor boxes generated using that position as a midpoint. It is not hard to see that, in essence, we use the information of the input image in a certain receptive field to predict the category and offset of the anchor boxes close to the field on the input image.

When the feature maps of different layers have receptive fields of different sizes on the input image, they are used to detect objects of different sizes. For example, we can design a network to have a wider receptive field for each unit in the feature map that is closer to the output layer, to detect objects with larger sizes in the input image.

We will implement a multiscale object detection model in the following section.

### 14.5.1 Summary

- We can generate anchor boxes with different numbers and sizes on multiple scales to detect objects of different sizes on multiple scales.
- The shape of the feature map can be used to determine the midpoint of the anchor boxes that uniformly sample any image.
- We use the information for the input image from a certain receptive field to predict the category and offset of the anchor boxes close to that field on the image.

### 14.5.2 Exercises

- Given an input image, assume  $1 \times c_i \times h \times w$  to be the shape of the feature map while  $c_i, h, w$  are the number, height, and width of the feature map. What methods can you think of to convert this variable into the anchor box's category and offset? What is the shape of the output?

### 14.5.3 Scan the QR Code to Discuss<sup>181</sup>



## 14.6 Object Detection Data Set (Pikachu)

There are no small data sets, like MNIST or Fashion-MNIST, in the object detection field. In order to quickly test models, we are going to assemble a small data set. First, we generate 1000 Pikachu images of different angles and sizes using an open source 3D Pikachu model. Then, we collect a series of background

<sup>181</sup> <https://discuss.mxnet.io/t/2446>

images and place a Pikachu image at a random position on each image. We use the `im2rec` tool<sup>182</sup> provided by MXNet to convert the images to binary RecordIO format[1]. This format can reduce the storage overhead of the data set on the disk and improve the reading efficiency. If you want to learn more about how to read images, refer to the documentation for the `GluonCV Toolkit`<sup>183</sup>.

### 14.6.1 Download the Data Set

The Pikachu data set in RecordIO format can be downloaded directly from the Internet. The operation for downloading the data set is defined in the function `_download_pikachu`.

```
%matplotlib inline
import d2l
from mxnet import gluon, image
import os

# Save to the d2l package.
def download_pikachu(data_dir):
    root_url = ('https://apache-mxnet.s3-accelerate.amazonaws.com/'
                'gluon/dataset/pikachu/')
    dataset = {'train.rec': 'e6bcb6ffba1ac04ff8a9b1115e650af56ee969c8',
               'train.idx': 'dcf7318b2602c06428b9988470c731621716c393',
               'val.rec': 'd6c33f799b4d058e82f2cb5bd9a976f69d72d520'}
    for k, v in dataset.items():
        gluon.utils.download(
            root_url + k, os.path.join(data_dir, k), sha1_hash=v)
```

### 14.6.2 Read the Data Set

We are going to read the object detection data set by creating the instance `ImageDetIter`. The “Det” in the name refers to Detection. We will read the training data set in random order. Since the format of the data set is RecordIO, we need the image index file '`train.idx`' to read random mini-batches. In addition, for each image of the training set, we will use random cropping and require the cropped image to cover at least 95% of each object. Since the cropping is random, this requirement is not always satisfied. We preset the maximum number of random cropping attempts to 200. If none of them meets the requirement, the image will not be cropped. To ensure the certainty of the output, we will not randomly crop the images in the test data set. We also do not need to read the test data set in random order.

```
# Save to the d2l package.
def load_data_pikachu(batch_size, edge_size=256):
    """Load the pikachu dataset"""
    data_dir = '../data/pikachu'
    download_pikachu(data_dir)
    train_iter = image.ImageDetIter(
        path_imgrec=os.path.join(data_dir, 'train.rec'),
        path_imgidx=os.path.join(data_dir, 'train.idx'),
        batch_size=batch_size,
        data_shape=(3, edge_size, edge_size), # The shape of the output image
        shuffle=True, # Read the data set in random order
        rand_crop=1, # The probability of random cropping is 1
```

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<sup>182</sup> <https://github.com/apache/incubator-mxnet/blob/master/tools/im2rec.py>

<sup>183</sup> <https://gluon-cv.mxnet.io/>

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```

    min_object_covered=0.95, max_attempts=200)
val_iter = image.ImageDetIter(
    path_imgrec=os.path.join(data_dir, 'val.rec'), batch_size=batch_size,
    data_shape=(3, edge_size, edge_size), shuffle=False)
return train_iter, val_iter

```

Below, we read a mini-batch and print the shape of the image and label. The shape of the image is the same as in the previous experiment (batch size, number of channels, height, width). The shape of the label is (batch size,  $m$ , 5), where  $m$  is equal to the maximum number of bounding boxes contained in a single image in the data set. Although computation for the mini-batch is very efficient, it requires each image to contain the same number of bounding boxes so that they can be placed in the same batch. Since each image may have a different number of bounding boxes, we can add illegal bounding boxes to images that have less than  $m$  bounding boxes until each image contains  $m$  bounding boxes. Thus, we can read a mini-batch of images each time. The label of each bounding box in the image is represented by an array of length 5. The first element in the array is the category of the object contained in the bounding box. When the value is -1, the bounding box is an illegal bounding box for filling purpose. The remaining four elements of the array represent the  $x, y$  axis coordinates of the upper-left corner of the bounding box and the  $x, y$  axis coordinates of the lower-right corner of the bounding box (the value range is between 0 and 1). The Pikachu data set here has only one bounding box per image, so  $m = 1$ .

```

batch_size, edge_size = 32, 256
train_iter, _ = load_data_pikachu(batch_size, edge_size)
batch = train_iter.next()
batch.data[0].shape, batch.label[0].shape

```

```
((32, 3, 256, 256), (32, 1, 5))
```

### 14.6.3 Graphic Data

We have ten images with bounding boxes on them. We can see that the angle, size, and position of Pikachu are different in each image. Of course, this is a simple man-made data set. In actual practice, the data is usually much more complicated.

```

imgs = (batch.data[0][0:10].transpose((0, 2, 3, 1))) / 255
axes = d2l.show_images(imgs, 2, 5, scale=2)
for ax, label in zip(axes, batch.label[0][0:10]):
    d2l.show_bboxes(ax, [label[0][1:5] * edge_size], colors=['w'])

```



#### 14.6.4 Summary

- The Pikachu data set we synthesized can be used to test object detection models.
- The data reading for object detection is similar to that for image classification. However, after we introduce bounding boxes, the label shape and image augmentation (e.g., random cropping) are changed.

#### 14.6.5 Exercises

- Referring to the MXNet documentation, what are the parameters for the constructors of the `image.ImageDetIter` and `image.CreateDetAugmenter` classes? What is their significance?

#### 14.6.6 Scan the QR Code to Discuss<sup>184</sup>



## 14.7 Single Shot Multibox Detection (SSD)

In the previous few sections, we have introduced bounding boxes, anchor boxes, multiscale object detection, and data sets. Now, we will use this background knowledge to construct an object detection model: single shot multibox detection (SSD) [40]. This quick and easy model is already widely used. Some of the design concepts and implementation details of this model are also applicable to other object detection models.

---

<sup>184</sup> <https://discuss.mxnet.io/t/2452>

### 14.7.1 Model

Fig. 14.7.1 shows the design of an SSD model. The model's main components are a base network block and several multiscale feature blocks connected in a series. Here, the base network block is used to extract features of original images, and it generally takes the form of a deep convolutional neural network. The paper on SSDs chooses to place a truncated VGG before the classification layer [40], but this is now commonly replaced by ResNet. We can design the base network so that it outputs larger heights and widths. In this way, more anchor boxes are generated based on this feature map, allowing us to detect smaller objects. Next, each multiscale feature block reduces the height and width of the feature map provided by the previous layer (for example, it may reduce the sizes by half). The blocks then use each element in the feature map to expand the receptive field on the input image. In this way, the closer a multiscale feature block is to the top of Fig. 14.7.1 the smaller its output feature map, and the fewer the anchor boxes that are generated based on the feature map. In addition, the closer a feature block is to the top, the larger the receptive field of each element in the feature map and the better suited it is to detect larger objects. As the SSD generates different numbers of anchor boxes of different sizes based on the base network block and each multiscale feature block and then predicts the categories and offsets (i.e., predicted bounding boxes) of the anchor boxes in order to detect objects of different sizes, SSD is a multiscale object detection model.

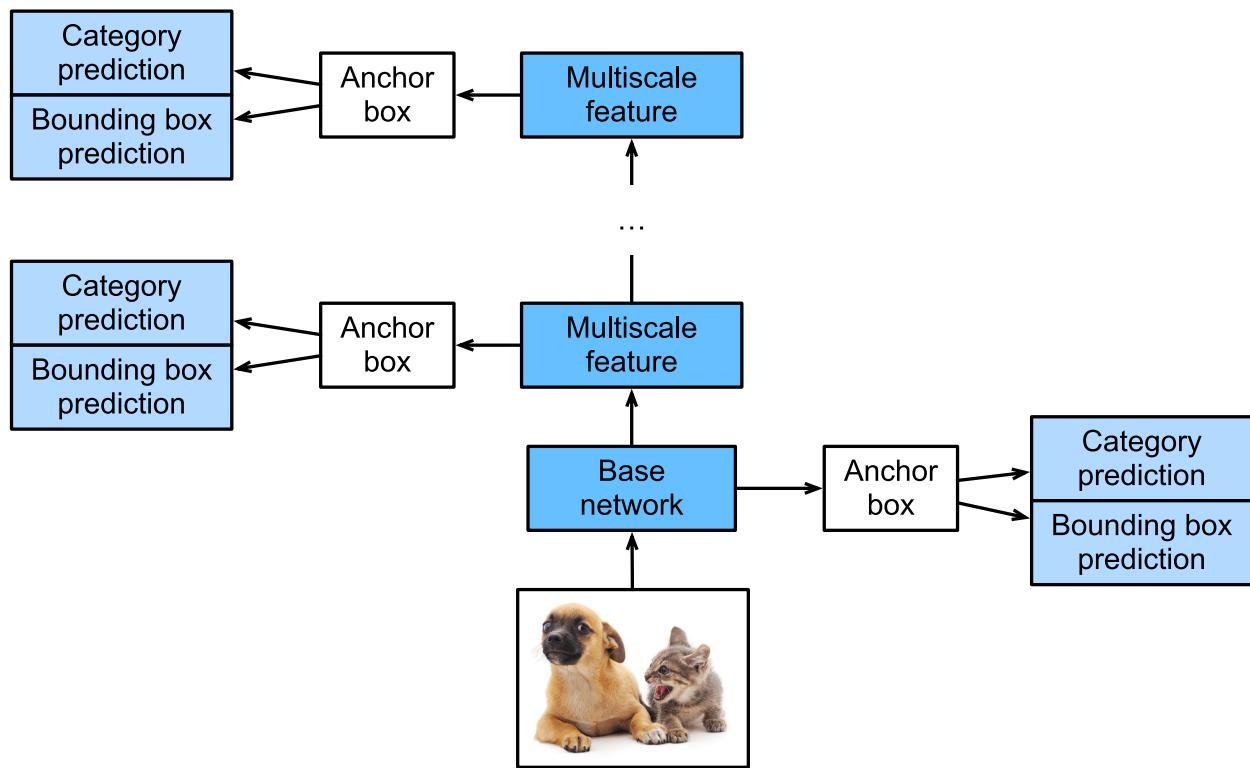


Fig. 14.7.1: The SSD is composed of a base network block and several multiscale feature blocks connected in a series.

Next, we will describe the implementation of the modules in Fig. 14.7.1. First, we need to discuss the implementation of category prediction and bounding box prediction.

#### Category Prediction Layer

Set the number of object categories to  $q$ . In this case, the number of anchor box categories is  $q + 1$ , with 0 indicating an anchor box that only contains background. For a certain scale, set the height and width of the feature map to  $h$  and  $w$ , respectively. If we use each element as the center to generate  $a$  anchor boxes, we

need to classify a total of  $hwa$  anchor boxes. If we use a fully connected layer (FCN) for the output, this will likely result in an excessive number of model parameters. Recall how we used convolutional layer channels to output category predictions in [Section 9.3](#). SSD uses the same method to reduce the model complexity.

Specifically, the category prediction layer uses a convolutional layer that maintains the input height and width. Thus, the output and input have a one-to-one correspondence to the spatial coordinates along the width and height of the feature map. Assuming that the output and input have the same spatial coordinates  $(x, y)$ , the channel for the coordinates  $(x, y)$  on the output feature map contains the category predictions for all anchor boxes generated using the input feature map coordinates  $(x, y)$  as the center. Therefore, there are  $a(q + 1)$  output channels, with the output channels indexed as  $i(q + 1) + j$  ( $0 \leq j \leq q$ ) representing the predictions of the category index  $j$  for the anchor box index  $i$ .

Now, we will define a category prediction layer of this type. After we specify the parameters  $a$  and  $q$ , it uses a  $3 \times 3$  convolutional layer with a padding of 1. The heights and widths of the input and output of this convolutional layer remain unchanged.

```
%matplotlib inline
import d2l
from mxnet import autograd, contrib, gluon, image, init, nd
from mxnet.gluon import nn

def cls_predictor(num_anchors, num_classes):
    return nn.Conv2D(num_anchors * (num_classes + 1), kernel_size=3,
                   padding=1)
```

## Bounding Box Prediction Layer

The design of the bounding box prediction layer is similar to that of the category prediction layer. The only difference is that, here, we need to predict 4 offsets for each anchor box, rather than  $q + 1$  categories.

```
def bbox_predictor(num_anchors):
    return nn.Conv2D(num_anchors * 4, kernel_size=3, padding=1)
```

## Concatenating Predictions for Multiple Scales

As we mentioned, SSD uses feature maps based on multiple scales to generate anchor boxes and predict their categories and offsets. Because the shapes and number of anchor boxes centered on the same element differ for the feature maps of different scales, the prediction outputs at different scales may have different shapes.

In the following example, we use the same batch of data to construct feature maps of two different scales,  $Y_1$  and  $Y_2$ . Here,  $Y_2$  has half the height and half the width of  $Y_1$ . Using category prediction as an example, we assume that each element in the  $Y_1$  and  $Y_2$  feature maps generates five ( $Y_1$ ) or three ( $Y_2$ ) anchor boxes. When there are 10 object categories, the number of category prediction output channels is either  $5 \times (10 + 1) = 55$  or  $3 \times (10 + 1) = 33$ . The format of the prediction output is (batch size, number of channels, height, width). As you can see, except for the batch size, the sizes of the other dimensions are different. Therefore, we must transform them into a consistent format and concatenate the predictions of the multiple scales to facilitate subsequent computation.

```
def forward(x, block):
    block.initialize()
    return block(x)

Y1 = forward(nd.zeros((2, 8, 20, 20)), cls_predictor(5, 10))
```

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```
Y2 = forward(nd.zeros((2, 16, 10, 10)), cls_predictor(3, 10))
(Y1.shape, Y2.shape)
```

```
((2, 55, 20, 20), (2, 33, 10, 10))
```

The channel dimension contains the predictions for all anchor boxes with the same center. We first move the channel dimension to the final dimension. Because the batch size is the same for all scales, we can convert the prediction results to binary format (batch size, height  $\times$  width  $\times$  number of channels) to facilitate subsequent concatenation on the 1st dimension.

```
def flatten_pred(pred):
    return pred.transpose((0, 2, 3, 1)).flatten()

def concat_preds(preds):
    return nd.concat(*[flatten_pred(p) for p in preds], dim=1)
```

Thus, regardless of the different shapes of  $Y_1$  and  $Y_2$ , we can still concatenate the prediction results for the two different scales of the same batch.

```
concat_preds([Y1, Y2]).shape
```

```
(2, 25300)
```

## Height and Width Downsample Block

For multiscale object detection, we define the following `down_sample_blk` block, which reduces the height and width by 50%. This block consists of two  $3 \times 3$  convolutional layers with a padding of 1 and a  $2 \times 2$  maximum pooling layer with a stride of 2 connected in a series. As we know,  $3 \times 3$  convolutional layers with a padding of 1 do not change the shape of feature maps. However, the subsequent pooling layer directly reduces the size of the feature map by half. Because  $1 \times 2 + (3 - 1) + (3 - 1) = 6$ , each element in the output feature map has a receptive field on the input feature map of the shape  $6 \times 6$ . As you can see, the height and width downsample block enlarges the receptive field of each element in the output feature map.

```
def down_sample_blk(num_channels):
    blk = nn.Sequential()
    for _ in range(2):
        blk.add(nn.Conv2D(num_channels, kernel_size=3, padding=1),
               nn.BatchNorm(in_channels=num_channels),
               nn.Activation('relu'))
    blk.add(nn.MaxPool2D(2))
    return blk
```

By testing forward computation in the height and width downsample block, we can see that it changes the number of input channels and halves the height and width.

```
forward(nd.zeros((2, 3, 20, 20)), down_sample_blk(10)).shape
```

```
(2, 10, 10, 10)
```

## Base Network Block

The base network block is used to extract features from original images. To simplify the computation, we will construct a small base network. This network consists of three height and width downsample blocks connected in a series, so it doubles the number of channels at each step. When we input an original image with the shape  $256 \times 256$ , the base network block outputs a feature map with the shape  $32 \times 32$ .

```
def base_net():
    blk = nn.Sequential()
    for num_filters in [16, 32, 64]:
        blk.add(down_sample_blk(num_filters))
    return blk

forward(nd.zeros((2, 3, 256, 256)), base_net()).shape
```

(2, 64, 32, 32)

## The Complete Model

The SSD model contains a total of five modules. Each module outputs a feature map used to generate anchor boxes and predict the categories and offsets of these anchor boxes. The first module is the base network block, modules two to four are height and width downsample blocks, and the fifth module is a global maximum pooling layer that reduces the height and width to 1. Therefore, modules two to five are all multiscale feature blocks shown in Fig. 14.7.1.

```
def get_blk(i):
    if i == 0:
        blk = base_net()
    elif i == 4:
        blk = nn.GlobalMaxPool2D()
    else:
        blk = down_sample_blk(128)
    return blk
```

Now, we will define the forward computation process for each module. In contrast to the previously-described convolutional neural networks, this module not only returns feature map Y output by convolutional computation, but also the anchor boxes of the current scale generated from Y and their predicted categories and offsets.

```
def blk_forward(X, blk, size, ratio, cls_predictor, bbox_predictor):
    Y = blk(X)
    anchors = contrib.ndarray.MultiBoxPrior(Y, sizes=size, ratios=ratio)
    cls_preds = cls_predictor(Y)
    bbox_preds = bbox_predictor(Y)
    return (Y, anchors, cls_preds, bbox_preds)
```

As we mentioned, the closer a multiscale feature block is to the top in Fig. 14.7.1, the larger the objects it detects and the larger the anchor boxes it must generate. Here, we first divide the interval from 0.2 to 1.05 into five equal parts to determine the sizes of smaller anchor boxes at different scales: 0.2, 0.37, 0.54, etc. Then, according to  $\sqrt{0.2 \times 0.37} = 0.272$ ,  $\sqrt{0.37 \times 0.54} = 0.447$ , and similar formulas, we determine the sizes of larger anchor boxes at the different scales.

```

sizes = [[0.2, 0.272], [0.37, 0.447], [0.54, 0.619], [0.71, 0.79],
         [0.88, 0.961]]
ratios = [[1, 2, 0.5]] * 5
num_anchors = len(sizes[0]) + len(ratios[0]) - 1

```

Now, we can define the complete model, TinySSD.

```

class TinySSD(nn.Block):
    def __init__(self, num_classes, **kwargs):
        super(TinySSD, self).__init__(**kwargs)
        self.num_classes = num_classes
        for i in range(5):
            # The assignment statement is self.blk_i = get_blk(i)
            setattr(self, 'blk_%d' % i, get_blk(i))
            setattr(self, 'cls_%d' % i, cls_predictor(num_anchors,
                                                       num_classes))
            setattr(self, 'bbox_%d' % i, bbox_predictor(num_anchors))

    def forward(self, X):
        anchors, cls_preds, bbox_preds = [None] * 5, [None] * 5, [None] * 5
        for i in range(5):
            # getattr(self, 'blk_%d' % i) accesses self.blk_i
            X, anchors[i], cls_preds[i], bbox_preds[i] = blk_forward(
                X, getattr(self, 'blk_%d' % i), sizes[i], ratios[i],
                getattr(self, 'cls_%d' % i), getattr(self, 'bbox_%d' % i))
        # In the reshape function, 0 indicates that the batch size remains
        # unchanged
        return (nd.concat(*anchors, dim=1),
                concat_preds(cls_preds).reshape(
                    (0, -1, self.num_classes + 1)), concat_preds(bbox_preds))

```

We now create an SSD model instance and use it to perform forward computation on image mini-batch  $X$ , which has a height and width of 256 pixels. As we verified previously, the first module outputs a feature map with the shape  $32 \times 32$ . Because modules two to four are height and width downsample blocks, module five is a global pooling layer, and each element in the feature map is used as the center for 4 anchor boxes, a total of  $(32^2 + 16^2 + 8^2 + 4^2 + 1) \times 4 = 5444$  anchor boxes are generated for each image at the five scales.

```

net = TinySSD(num_classes=1)
net.initialize()
X = nd.zeros((32, 3, 256, 256))
anchors, cls_preds, bbox_preds = net(X)

print('output anchors:', anchors.shape)
print('output class preds:', cls_preds.shape)
print('output bbox preds:', bbox_preds.shape)

```

```

output anchors: (1, 5444, 4)
output class preds: (32, 5444, 2)
output bbox preds: (32, 21776)

```

## 14.7.2 Training

Now, we will explain, step by step, how to train the SSD model for object detection.

### Data Reading and Initialization

We read the Pikachu data set we created in the previous section.

```
batch_size = 32
train_iter, _ = d2l.load_data_pikachu(batch_size)
```

There is 1 category in the Pikachu data set. After defining the module, we need to initialize the model parameters and define the optimization algorithm.

```
ctx, net = d2l.try_gpu(), TinySSD(num_classes=1)
net.initialize(init=init.Xavier(), ctx=ctx)
trainer = gluon.Trainer(net.collect_params(), 'sgd',
                        {'learning_rate': 0.2, 'wd': 5e-4})
```

### Define Loss and Evaluation Functions

Object detection is subject to two types of losses. The first is anchor box category loss. For this, we can simply reuse the cross-entropy loss function we used in image classification. The second loss is positive anchor box offset loss. Offset prediction is a normalization problem. However, here, we do not use the squared loss introduced previously. Rather, we use the  $L_1$  norm loss, which is the absolute value of the difference between the predicted value and the ground-truth value. The mask variable `bbox_masks` removes negative anchor boxes and padding anchor boxes from the loss calculation. Finally, we add the anchor box category and offset losses to find the final loss function for the model.

```
cls_loss = gluon.loss.SoftmaxCrossEntropyLoss()
bbox_loss = gluon.loss.L1Loss()

def calc_loss(cls_preds, cls_labels, bbox_preds, bbox_labels, bbox_masks):
    cls = cls_loss(cls_preds, cls_labels)
    bbox = bbox_loss(bbox_preds * bbox_masks, bbox_labels * bbox_masks)
    return cls + bbox
```

We can use the accuracy rate to evaluate the classification results. As we use the  $L_1$  norm loss, we will use the average absolute error to evaluate the bounding box prediction results.

```
def cls_eval(cls_preds, cls_labels):
    # Because the category prediction results are placed in the final
    # dimension, argmax must specify this dimension
    return (cls_preds.argmax(axis=-1) == cls_labels).sum().asscalar()

def bbox_eval(bbox_preds, bbox_labels, bbox_masks):
    return ((bbox_labels - bbox_preds) * bbox_masks).abs().sum().asscalar()
```

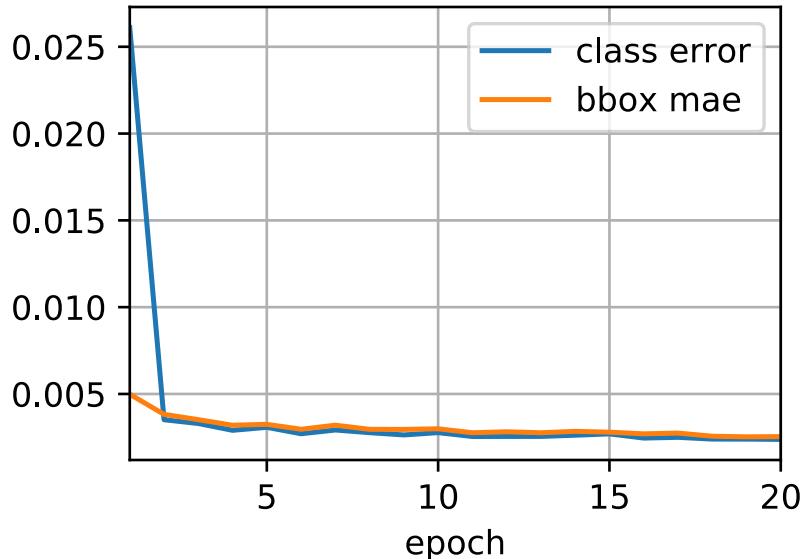
### Train the Model

During model training, we must generate multiscale anchor boxes (`anchors`) in the model's forward computation process and predict the category (`cls_preds`) and offset (`bbox_preds`) for each anchor box. Afterwards,

we label the category (`cls_labels`) and offset (`bbox_labels`) of each generated anchor box based on the label information `Y`. Finally, we calculate the loss function using the predicted and labeled category and offset values. To simplify the code, we do not evaluate the training data set here.

```
num_epochs, timer = 20, d2l.Timer()
animator = d2l.Animator(xlabel='epoch', xlim=[1, num_epochs],
                        legend=['class error', 'bbox mae'])
for epoch in range(num_epochs):
    # accuracy_sum, mae_sum, num_examples, num_labels
    metric = d2l.Accumulator(4)
    train_iter.reset() # Read data from the start.
    for batch in train_iter:
        timer.start()
        X = batch.data[0].as_in_context(ctx)
        Y = batch.label[0].as_in_context(ctx)
        with autograd.record():
            # Generate multiscale anchor boxes and predict the category and
            # offset of each
            anchors, cls_preds, bbox_preds = net(X)
            # Label the category and offset of each anchor box
            bbox_labels, bbox_masks, cls_labels = contrib.nd.MultiBoxTarget(
                anchors, Y, cls_preds.transpose((0, 2, 1)))
            # Calculate the loss function using the predicted and labeled
            # category and offset values
            l = calc_loss(cls_preds, cls_labels, bbox_preds, bbox_labels,
                          bbox_masks)
            l.backward()
            trainer.step(batch_size)
            metric.add(cls_eval(cls_preds, cls_labels), cls_labels.size,
                      bbox_eval(bbox_preds, bbox_labels, bbox_masks),
                      bbox_labels.size)
        cls_err, bbox_mae = 1-metric[0]/metric[1], metric[2]/metric[3]
        animator.add(epoch+1, (cls_err, bbox_mae))
print('class err %.2e, bbox mae %.2e' % (cls_err, bbox_mae))
print('%.1f examples/sec on %s'%(train_iter.num_image/timer.stop(), ctx))
```

```
class err 2.38e-03, bbox mae 2.54e-03
3981.4 examples/sec on gpu(0)
```



### 14.7.3 Prediction

In the prediction stage, we want to detect all objects of interest in the image. Below, we read the test image and transform its size. Then, we convert it to the four-dimensional format required by the convolutional layer.

```
img = image.imread('../img/pikachu.jpg')
feature = image.imresize(img, 256, 256).astype('float32')
X = feature.transpose((2, 0, 1)).expand_dims(axis=0)
```

Using the `MultiBoxDetection` function, we predict the bounding boxes based on the anchor boxes and their predicted offsets. Then, we use non-maximum suppression to remove similar bounding boxes.

```
def predict(X):
    anchors, cls_preds, bbox_preds = net(X.as_in_context(ctx))
    cls_probs = cls_preds.softmax().transpose((0, 2, 1))
    output = contrib.nd.MultiBoxDetection(cls_probs, bbox_preds, anchors)
    idx = [i for i, row in enumerate(output[0]) if row[0].asscalar() != -1]
    return output[0], idx

output = predict(X)
```

Finally, we take all the bounding boxes with a confidence level of at least 0.3 and display them as the final output.

```
def display(img, output, threshold):
    d2l.set_figsize((5, 5))
    fig = d2l.plt.imshow(img.asnumpy())
    for row in output:
        score = row[1].asscalar()
        if score < threshold:
            continue
        h, w = img.shape[0:2]
```

(continues on next page)

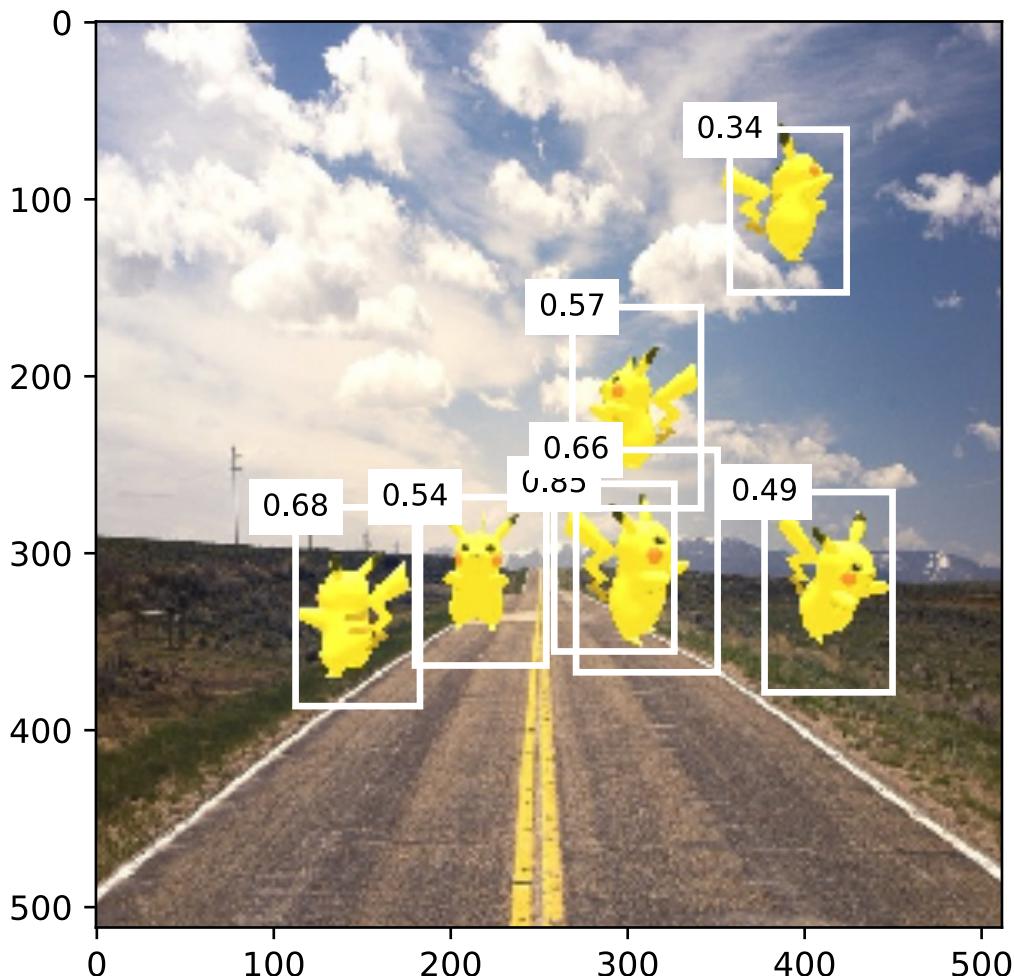
(continued from previous page)

```

bbox = [row[2:6] * nd.array((w, h, w, h), ctx=row.context)]
d2l.show_bboxes(fig.axes, bbox, '%.2f' % score, 'w')

display(img, output, threshold=0.3)

```



#### 14.7.4 Summary

- SSD is a multiscale object detection model. This model generates different numbers of anchor boxes of different sizes based on the base network block and each multiscale feature block and predicts the categories and offsets of the anchor boxes to detect objects of different sizes.
- During SSD model training, the loss function is calculated using the predicted and labeled category and offset values.

#### 14.7.5 Exercises

- Due to space limitations, we have ignored some of the implementation details of SSD models in this experiment. Can you further improve the model in the following areas?

## Loss Function

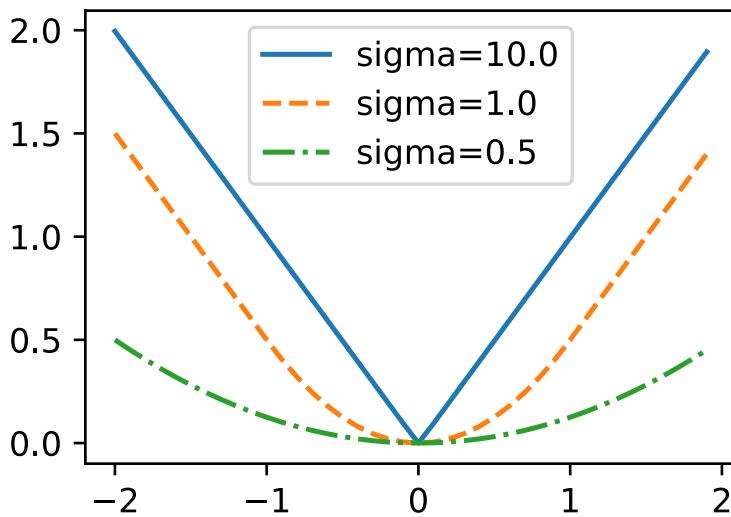
For the predicted offsets, replace  $L_1$  norm loss with  $L_1$  regularization loss. This loss function uses a square function around zero for greater smoothness. This is the regularized area controlled by the hyper-parameter  $\sigma$ :

$$f(x) = \begin{cases} (\sigma x)^2/2, & \text{if } |x| < 1/\sigma^2 \\ |x| - 0.5/\sigma^2, & \text{otherwise} \end{cases} \quad (14.7.1)$$

When  $\sigma$  is large, this loss is similar to the  $L_1$  norm loss. When the value is small, the loss function is smoother.

```
sigmas = [10, 1, 0.5]
lines = ['-', '--', '-.']
x = nd.arange(-2, 2, 0.1)
d2l.set_figsize()

for l, s in zip(lines, sigmas):
    y = nd.smooth_l1(x, scalar=s)
    d2l.plt.plot(x.asnumpy(), y.asnumpy(), l, label='sigma=%.1f' % s)
d2l.plt.legend();
```



In the experiment, we used cross-entropy loss for category prediction. Now, assume that the prediction probability of the actual category  $j$  is  $p_j$  and the cross-entropy loss is  $-\log p_j$ . We can also use the focal loss [37]. Given the positive hyper-parameters  $\gamma$  and  $\alpha$ , this loss is defined as:

$$-\alpha(1 - p_j)^\gamma \log p_j. \quad (14.7.2)$$

As you can see, by increasing  $\gamma$ , we can effectively reduce the loss when the probability of predicting the correct category is high.

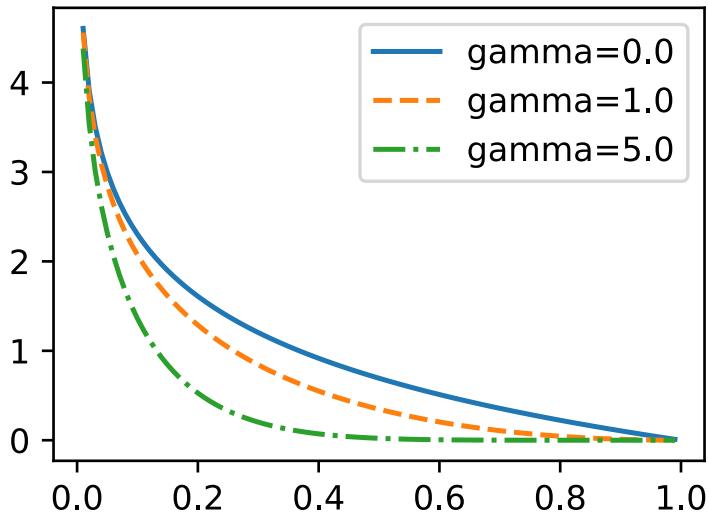
```
def focal_loss(gamma, x):
    return -(1 - x) ** gamma * x.log()

x = nd.arange(0.01, 1, 0.01)
for l, gamma in zip(lines, [0, 1, 5]):
```

(continues on next page)

(continued from previous page)

```
y = d21=plt.plot(x.asnumpy(), focal_loss(gamma, x).asnumpy(), 1,
                   label='gamma=%1f' % gamma)
d21=plt.legend();
```



### Training and Prediction

- When an object is relatively large compared to the image, the model normally adopts a larger input image size.
- This generally produces a large number of negative anchor boxes when labeling anchor box categories. We can sample the negative anchor boxes to better balance the data categories. To do this, we can set the `MultiBoxTarget` function's `negative_mining_ratio` parameter.
- Assign hyper-parameters with different weights to the anchor box category loss and positive anchor box offset loss in the loss function.
- Refer to the SSD paper. What methods can be used to evaluate the precision of object detection models [40]?

#### 14.7.6 Scan the QR Code to Discuss<sup>185</sup>



<sup>185</sup> <https://discuss.mxnet.io/t/2453>

## 14.8 Region-based CNNs (R-CNNs)

Region-based convolutional neural networks or regions with CNN features (R-CNNs) are a pioneering approach that applies deep models to object detection [17]. In this section, we will discuss R-CNNs and a series of improvements made to them: Fast R-CNN [Girshick.2015\*1], Faster R-CNN [16], and Mask R-CNN [21]. Due to space limitations, we will confine our discussion to the designs of these models.

### 14.8.1 R-CNNs

R-CNN models first select several proposed regions from an image (for example, anchor boxes are one type of selection method) and then label their categories and bounding boxes (e.g., offsets). Then, they use a CNN to perform forward computation to extract features from each proposed area. Afterwards, we use the features of each proposed region to predict their categories and bounding boxes. Fig. 14.8.1 shows an R-CNN model.

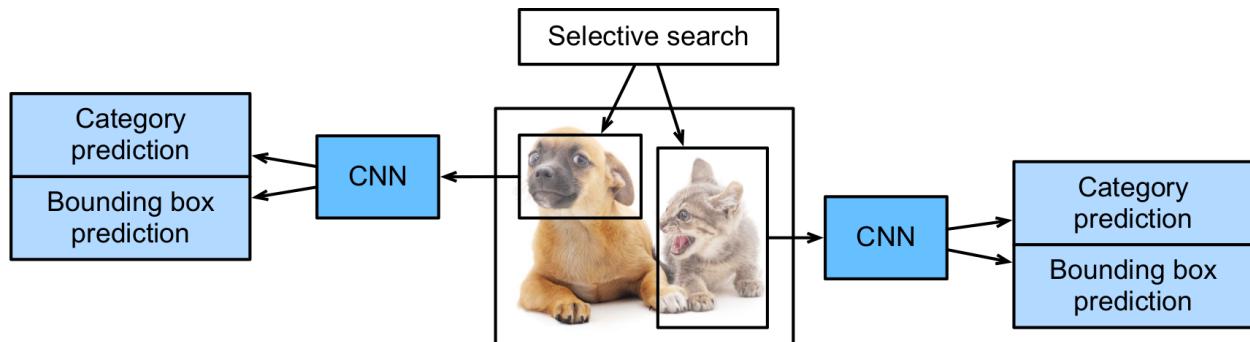


Fig. 14.8.1: R-CNN model.

Specifically, R-CNNs are composed of four main parts:

1. Selective search is performed on the input image to select multiple high-quality proposed regions [62]. These proposed regions are generally selected on multiple scales and have different shapes and sizes. The category and ground-truth bounding box of each proposed region is labeled.
2. A pre-trained CNN is selected and placed, in truncated form, before the output layer. It transforms each proposed region into the input dimensions required by the network and uses forward computation to output the features extracted from the proposed regions.
3. The features and labeled category of each proposed region are combined as an example to train multiple support vector machines for object classification. Here, each support vector machine is used to determine whether an example belongs to a certain category.
4. The features and labeled bounding box of each proposed region are combined as an example to train a linear regression model for ground-truth bounding box prediction.

Although R-CNN models use pre-trained CNNs to effectively extract image features, the main downside is the slow speed. As you can imagine, we can select thousands of proposed regions from a single image, requiring thousands of forward computations from the CNN to perform object detection. This massive computing load means that R-CNNs are not widely used in actual applications.

### 14.8.2 Fast R-CNN

The main performance bottleneck of an R-CNN model is the need to independently extract features for each proposed region. As these regions have a high degree of overlap, independent feature extraction results in

a high volume of repetitive computations. Fast R-CNN improves on the R-CNN by only performing CNN forward computation on the image as a whole.

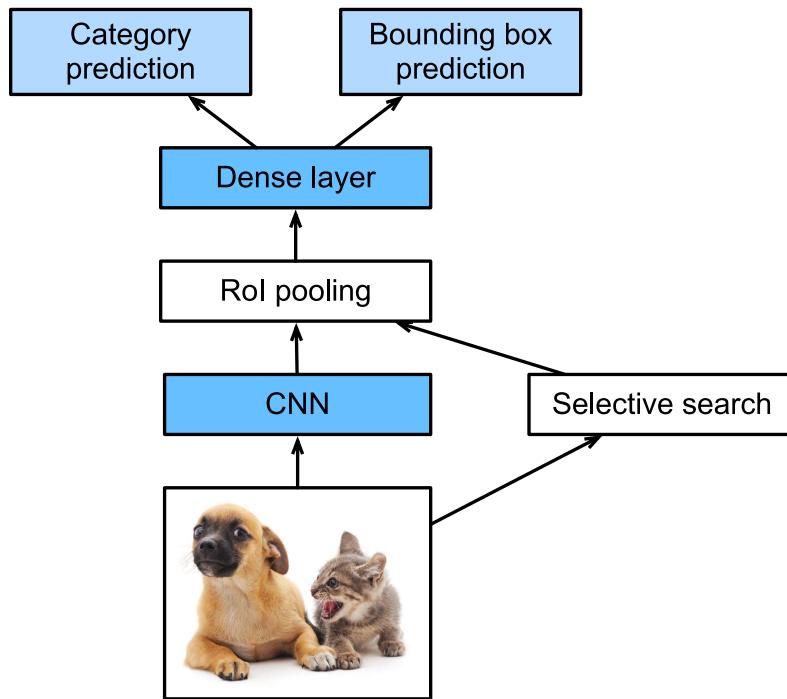


Fig. 14.8.2: Fast R-CNN model.

Fig. 14.8.2 shows a Fast R-CNN model. Its primary computation steps are described below:

1. Compared to an R-CNN model, a Fast R-CNN model uses the entire image as the CNN input for feature extraction, rather than each proposed region. Moreover, this network is generally trained to update the model parameters. As the input is an entire image, the CNN output shape is  $1 \times c \times h_1 \times w_1$ .
2. Assuming selective search generates  $n$  proposed regions, their different shapes indicate regions of interests (RoIs) of different shapes on the CNN output. Features of the same shapes must be extracted from these RoIs (here we assume that the height is  $h_2$  and the width is  $w_2$ ). Fast R-CNN introduces RoI pooling, which uses the CNN output and RoIs as input to output a concatenation of the features extracted from each proposed region with the shape  $n \times c \times h_2 \times w_2$ .
3. A fully connected layer is used to transform the output shape to  $n \times d$ , where  $d$  is determined by the model design.
4. During category prediction, the shape of the fully connected layer output is again transformed to  $n \times q$  and we use softmax regression ( $q$  is the number of categories). During bounding box prediction, the shape of the fully connected layer output is again transformed to  $n \times 4$ . This means that we predict the category and bounding box for each proposed region.

The RoI pooling layer in Fast R-CNN is somewhat different from the pooling layers we have discussed before. In a normal pooling layer, we set the pooling window, padding, and stride to control the output shape. In an RoI pooling layer, we can directly specify the output shape of each region, such as specifying the height and width of each region as  $h_2, w_2$ . Assuming that the height and width of the RoI window are  $h$  and  $w$ , this window is divided into a grid of sub-windows with the shape  $h_2 \times w_2$ . The size of each sub-window is about  $(h/h_2) \times (w/w_2)$ . The sub-window height and width must always be integers and the largest element is used as the output for a given sub-window. This allows the RoI pooling layer to extract features of the same shape from RoIs of different shapes.

In Fig. 14.8.3, we select an  $3 \times 3$  region as an ROI of the  $4 \times 4$  input. For this ROI, we use a  $2 \times 2$  ROI pooling layer to obtain a single  $2 \times 2$  output. When we divide the region into four sub-windows, they respectively contain the elements 0, 1, 4, and 5 (5 is the largest); 2 and 6 (6 is the largest); 8 and 9 (9 is the largest); and 10.

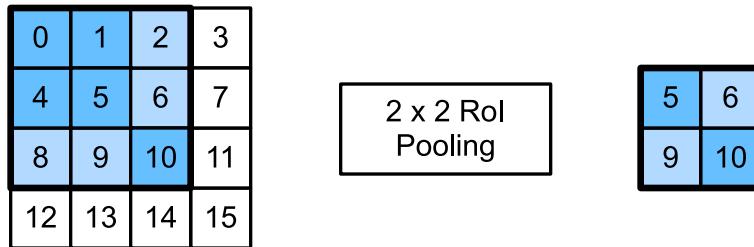


Fig. 14.8.3:  $2 \times 2$  ROI pooling layer.

We use the `ROIPooling` function to demonstrate the ROI pooling layer computation. Assume that the CNN extracts the feature  $X$  with both a height and width of 4 and only a single channel.

```
from mxnet import nd

X = nd.arange(16).reshape((1, 1, 4, 4))
X
```

```
[[[[ 0.  1.  2.  3.]
   [ 4.  5.  6.  7.]
   [ 8.  9.  10. 11.]
   [12. 13. 14. 15.]]]]
<NDArray 1x1x4x4 @cpu(0)>
```

Assume that the height and width of the image are both 40 pixels and that selective search generates two proposed regions on the image. Each region is expressed as five elements: the region's object category and the  $x, y$  coordinates of its upper-left and bottom-right corners.

```
rois = nd.array([[0, 0, 0, 20, 20], [0, 0, 10, 30, 30]])
```

Because the height and width of  $X$  are 1/10 of the height and width of the image, the coordinates of the two proposed regions are multiplied by 0.1 according to the `spatial_scale`, and then the ROIs are labeled on  $X$  as  $X[:, :, 0:3, 0:3]$  and  $X[:, :, 1:4, 0:4]$ , respectively. Finally, we divide the two ROIs into a sub-window grid and extract features with a height and width of 2.

```
nd.ROIPooling(X, rois, pooled_size=(2, 2), spatial_scale=0.1)
```

```
[[[[ 5.  6.]
   [ 9. 10.]]

 [[[ 9. 11.]
   [13. 15.]]]]
<NDArray 2x1x2x2 @cpu(0)>
```

### 14.8.3 Faster R-CNN

In order to obtain precise object detection results, Fast R-CNN generally requires that many proposed regions be generated in selective search. Faster R-CNN replaces selective search with a region proposal network. This reduces the number of proposed regions generated, while ensuring precise object detection.

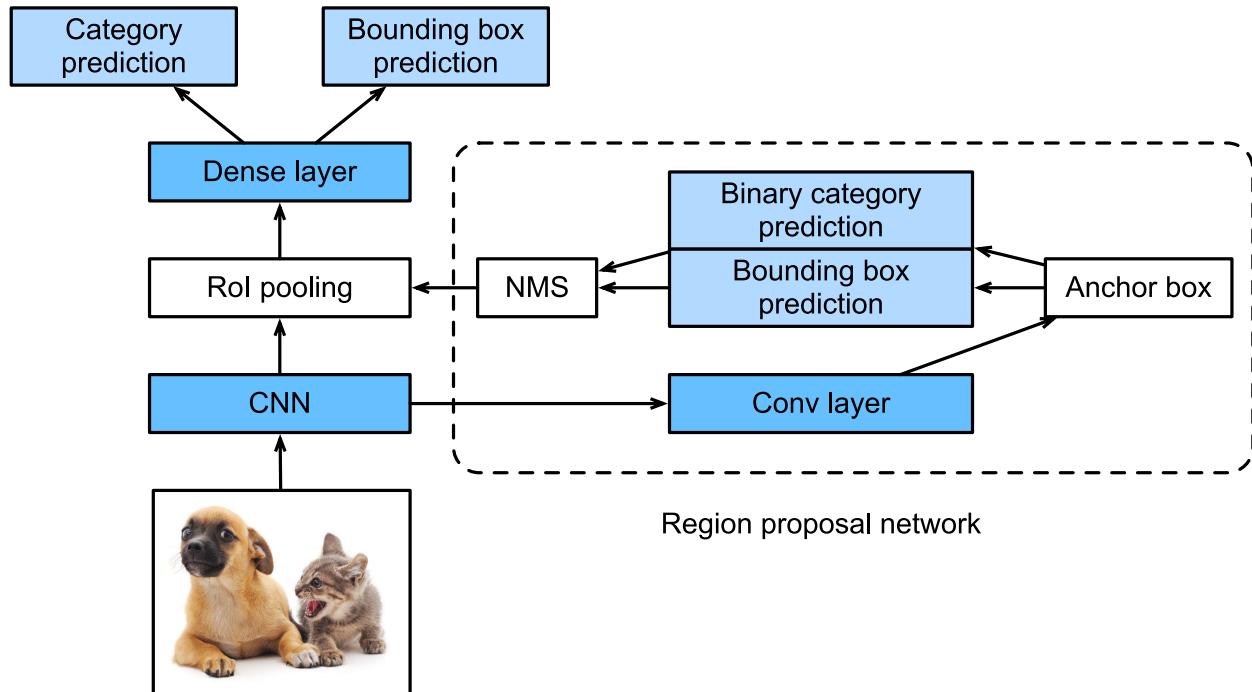


Fig. 14.8.4: Faster R-CNN model.

Fig. 14.8.4 shows a Faster R-CNN model. Compared to Fast R-CNN, Faster R-CNN only changes the method for generating proposed regions from selective search to region proposal network. The other parts of the model remain unchanged. The detailed region proposal network computation process is described below:

1. We use a  $3 \times 3$  convolutional layer with a padding of 1 to transform the CNN output and set the number of output channels to  $c$ . This way, each element in the feature map the CNN extracts from the image is a new feature with a length of  $c$ .
2. We use each element in the feature map as a center to generate multiple anchor boxes of different sizes and aspect ratios and then label them.
3. We use the features of the elements of length  $c$  at the center on the anchor boxes to predict the binary category (object or background) and bounding box for their respective anchor boxes.
4. Then, we use non-maximum suppression to remove similar bounding box results that correspond to category predictions of “object”. Finally, we output the predicted bounding boxes as the proposed regions required by the ROI pooling layer.

It is worth noting that, as a part of the Faster R-CNN model, the region proposal network is trained together with the rest of the model. In addition, the Faster R-CNN object functions include the category and bounding box predictions in object detection, as well as the binary category and bounding box predictions for the anchor boxes in the region proposal network. Finally, the region proposal network can learn how to generate high-quality proposed regions, which reduces the number of proposed regions while maintaining the precision of object detection.

#### 14.8.4 Mask R-CNN

If training data is labeled with the pixel-level positions of each object in an image, a Mask R-CNN model can effectively use these detailed labels to further improve the precision of object detection.

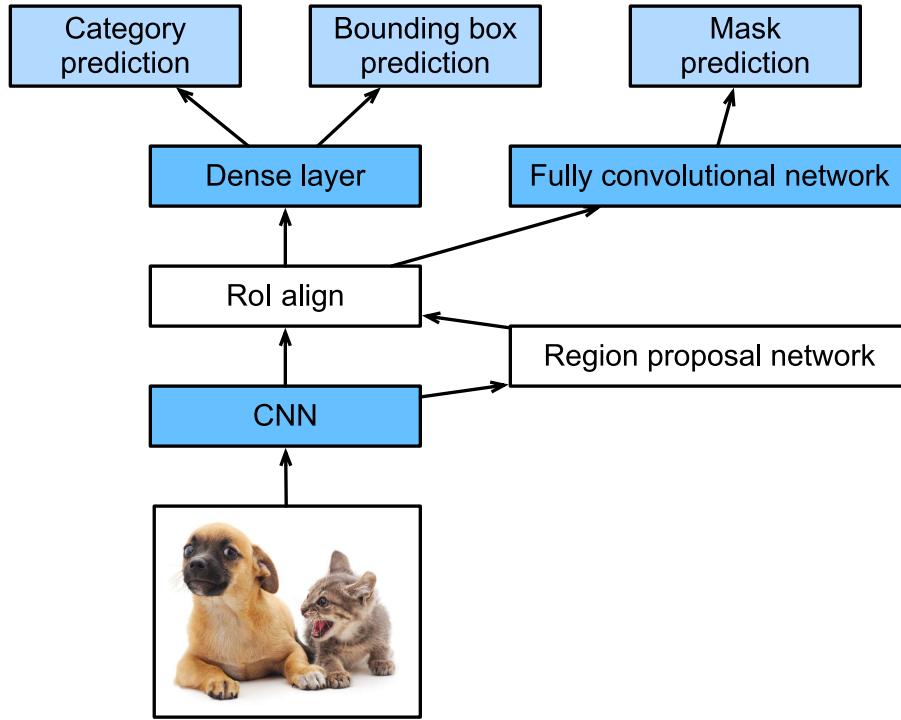


Fig. 14.8.5: Mask R-CNN model.

As shown in Fig. 14.8.5, Mask R-CNN is a modification to the Faster R-CNN model. Mask R-CNN models replace the RoI pooling layer with an RoI alignment layer. This allows the use of bilinear interpolation to retain spatial information on feature maps, making Mask R-CNN better suited for pixel-level predictions. The RoI alignment layer outputs feature maps of the same shape for all RoIs. This not only predicts the categories and bounding boxes of RoIs, but allows us to use an additional fully convolutional network to predict the pixel-level positions of objects. We will describe how to use fully convolutional networks to predict pixel-level semantics in images later in this chapter.

#### 14.8.5 Summary

- An R-CNN model selects several proposed regions and uses a CNN to perform forward computation and extract the features from each proposed region. It then uses these features to predict the categories and bounding boxes of proposed regions.
- Fast R-CNN improves on the R-CNN by only performing CNN forward computation on the image as a whole. It introduces an RoI pooling layer to extract features of the same shape from RoIs of different shapes.
- Faster R-CNN replaces the selective search used in Fast R-CNN with a region proposal network. This reduces the number of proposed regions generated, while ensuring precise object detection.
- Mask R-CNN uses the same basic structure as Faster R-CNN, but adds a fully convolution layer to help locate objects at the pixel level and further improve the precision of object detection.

### 14.8.6 Exercises

- Study the implementation of each model in the GluonCV toolkit<sup>186</sup> related to this section.

### 14.8.7 Scan the QR Code to Discuss<sup>187</sup>



## 14.9 Semantic Segmentation and Data Sets

In our discussion of object detection issues in the previous sections, we only used rectangular bounding boxes to label and predict objects in images. In this section, we will look at semantic segmentation, which attempts to segment images into regions with different semantic categories. These semantic regions label and predict objects at the pixel level. Figure 11.10 shows a semantically-segmented image, with areas labeled “dog”, “cat”, and “background”. As you can see, compared to object detection, semantic segmentation labels areas with pixel-level borders, for significantly greater precision.



Fig. 14.9.1: Semantically-segmented image, with areas labeled “dog”, “cat”, and “background”.

### 14.9.1 Image Segmentation and Instance Segmentation

In the computer vision field, there are two important methods related to semantic segmentation: image segmentation and instance segmentation. Here, we will distinguish these concepts from semantic segmentation as follows:

- Image segmentation divides an image into several constituent regions. This method generally uses the correlations between pixels in an image. During training, labels are not needed for image pixels. However, during prediction, this method cannot ensure that the segmented regions have the semantics we want. If we input the image in 9.10, image segmentation might divide the dog into two regions, one

<sup>186</sup> <https://github.com/dmlc/gluon-cv/>

<sup>187</sup> <https://discuss.mxnet.io/t/2447>

covering the dog's mouth and eyes where black is the prominent color and the other covering the rest of the dog where yellow is the prominent color.

- Instance segmentation is also called simultaneous detection and segmentation. This method attempts to identify the pixel-level regions of each object instance in an image. In contrast to semantic segmentation, instance segmentation not only distinguishes semantics, but also different object instances. If an image contains two dogs, instance segmentation will distinguish which pixels belong to which dog.

## 14.9.2 Pascal VOC2012 Semantic Segmentation Data Set

In the semantic segmentation field, one important data set is Pascal VOC2012<sup>188</sup>. To better understand this data set, we must first import the package or module needed for the experiment.

```
%matplotlib inline
import d2l
from mxnet import gluon, image, nd
import os
import tarfile
```

The original site might be unstable, we download the data from a mirror site. We download the archive to the `../data` path. The archive is about 2GB, so it will take some time to download. After you decompress the archive, the data set is located in the `../data/VOCdevkit/VOC2012` path.

```
# Save to the d2l package.
def download_voc_pascal(data_dir='../data'):
    """Download the VOC2012 segmentation dataset."""
    voc_dir = os.path.join(data_dir, 'VOCdevkit/VOC2012')
    url = ('http://data.mxnet.io/data/VOCtrainval_11-May-2012.tar')
    sha1 = '4e443f8a2eca6b1dac8a6c57641b67dd40621a49'
    fname = gluon.utils.download(url, data_dir, sha1_hash=sha1)
    with tarfile.open(fname, 'r') as f:
        f.extractall(data_dir)
    return voc_dir

voc_dir = download_voc_pascal()
```

Go to `../data/VOCdevkit/VOC2012` to see the different parts of the data set. The `ImageSets/Segmentation` path contains text files that specify the training and testing examples. The `JPEGImages` and `SegmentationClass` paths contain the example input images and labels, respectively. These labels are also in image format, with the same dimensions as the input images to which they correspond. In the labels, pixels with the same color belong to the same semantic category. The `read_voc_images` function defined below reads all input images and labels to the memory.

```
# Save to the d2l package.
def read_voc_images(root='../../data/VOCdevkit/VOC2012', is_train=True):
    """Read all VOC feature and label images."""
    txt_fname = '%s/ImageSets/Segmentation/%s' % (
        root, 'train.txt' if is_train else 'val.txt')
    with open(txt_fname, 'r') as f:
        images = f.read().split()
    features, labels = [None] * len(images), [None] * len(images)
    for i, fname in enumerate(images):
```

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<sup>188</sup> <http://host.robots.ox.ac.uk/pascal/VOC/voc2012/>

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```

features[i] = image.imread('%s/JPEGImages/%s.jpg' % (root, fname))
labels[i] = image.imread(
    '%s/SegmentationClass/%s.png' % (root, fname))
return features, labels

train_features, train_labels = read_voc_images(voc_dir, True)

```

We draw the first five input images and their labels. In the label images, white represents borders and black represents the background. Other colors correspond to different categories.

```

n = 5
imgs = train_features[0:n] + train_labels[0:n]
d2l.show_images(imgs, 2, n);

```



Next, we list each RGB color value in the labels and the categories they label.

```

# Save to the d2l package.
VOC_COLORMAP = [[0, 0, 0], [128, 0, 0], [0, 128, 0], [128, 128, 0],
                 [0, 0, 128], [128, 0, 128], [0, 128, 128], [128, 128, 128],
                 [64, 0, 0], [192, 0, 0], [64, 128, 0], [192, 128, 0],
                 [64, 0, 128], [192, 0, 128], [64, 128, 128], [192, 128, 128],
                 [0, 64, 0], [128, 64, 0], [0, 192, 0], [128, 192, 0],
                 [0, 64, 128]]
# Save to the d2l package.
VOC_CLASSES = ['background', 'aeroplane', 'bicycle', 'bird', 'boat',
                'bottle', 'bus', 'car', 'cat', 'chair', 'cow',
                'diningtable', 'dog', 'horse', 'motorbike', 'person',
                'potted plant', 'sheep', 'sofa', 'train', 'tv/monitor']

```

After defining the two constants above, we can easily find the category index for each pixel in the labels.

```

# Save to the d2l package.
def build_colormap2label():
    """Build a RGB color to label mapping for segmentation."""
    colormap2label = nd.zeros(256 ** 3)
    for i, colormap in enumerate(VOC_COLORMAP):
        colormap2label[(colormap[0]*256 + colormap[1])*256 + colormap[2]] = i
    return colormap2label

```

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```
# Save to the d2l package.
def voc_label_indices(colormap, colormap2label):
    """Map a RGB color to a label."""
    colormap = colormap.astype('int32')
    idx = ((colormap[:, :, 0] * 256 + colormap[:, :, 1]) * 256
           + colormap[:, :, 2])
    return colormap2label[idx]
```

For example, in the first example image, the category index for the front part of the airplane is 1 and the index for the background is 0.

```
y = voc_label_indices(train_labels[0], build_colormap2label())
y[105:115, 130:140], VOC_CLASSES[1]
```

```
([[0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]
 [0. 0. 0. 0. 0. 0. 0. 1. 1. 1.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1.]
 [0. 0. 0. 0. 0. 1. 1. 1. 1. 1.]
 [0. 0. 0. 0. 0. 1. 1. 1. 1. 1.]
 [0. 0. 0. 0. 1. 1. 1. 1. 1. 1.]
 [0. 0. 0. 0. 1. 1. 1. 1. 1. 1.]
 [0. 0. 0. 0. 1. 1. 1. 1. 1. 1.]
 [0. 0. 0. 0. 0. 1. 1. 1. 1. 1.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1.]
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]]
<NDArray 10x10 @cpu(0)>, 'aeroplane')
```

## Data Preprocessing

In the preceding chapters, we scaled images to make them fit the input shape of the model. In semantic segmentation, this method would require us to re-map the predicted pixel categories back to the original-size input image. It would be very difficult to do this precisely, especially in segmented regions with different semantics. To avoid this problem, we crop the images to set dimensions and do not scale them. Specifically, we use the random cropping method used in image augmentation to crop the same region from input images and their labels.

```
# Save to the d2l package.
def voc_rand_crop(feature, label, height, width):
    """Randomly crop for both feature and label images."""
    feature, rect = image.random_crop(feature, (width, height))
    label = image.fixed_crop(label, *rect)
    return feature, label

imgs = []
for _ in range(n):
    imgs += voc_rand_crop(train_features[0], train_labels[0], 200, 300)
d2l.show_images(imgs[::2] + imgs[1::2], 2, n);
```



### Data Set Classes for Custom Semantic Segmentation

We use the inherited `Dataset` class provided by Gluon to customize the semantic segmentation data set class `VOCSegDataset`. By implementing the `__getitem__` function, we can arbitrarily access the input image with the index `idx` and the category indexes for each of its pixels from the data set. As some images in the data set may be smaller than the output dimensions specified for random cropping, we must remove these example by using a custom `filter` function. In addition, we define the `normalize_image` function to normalize each of the three RGB channels of the input images.

```
# Save to the d2l package.
class VOCSegDataset(gluon.data.Dataset):
    """A customized dataset to load VOC dataset."""
    def __init__(self, is_train, crop_size, voc_dir):
        self.rgb_mean = nd.array([0.485, 0.456, 0.406])
        self.rgb_std = nd.array([0.229, 0.224, 0.225])
        self.crop_size = crop_size
        features, labels = read_voc_images(root=voc_dir, is_train=is_train)
        self.features = [self.normalize_image(feature)
                         for feature in self.filter(features)]
        self.labels = self.filter(labels)
        self.colormap2label = build_colormap2label()
        print('read ' + str(len(self.features)) + ' examples')

    def normalize_image(self, img):
        return (img.astype('float32') / 255 - self.rgb_mean) / self.rgb_std

    def filter(self, imgs):
        return [img for img in imgs if (
            img.shape[0] >= self.crop_size[0] and
            img.shape[1] >= self.crop_size[1])]

    def __getitem__(self, idx):
        feature, label = voc_rand_crop(self.features[idx], self.labels[idx],
                                         *self.crop_size)
        return (feature.transpose((2, 0, 1)),
                voc_label_indices(label, self.colormap2label))

    def __len__(self):
        return len(self.features)
```

## Read the Data Set

Using the custom `VOCSegDataset` class, we create the training set and testing set instances. We assume the random cropping operation output images in the shape  $320 \times 480$ . Below, we can see the number of examples retained in the training and testing sets.

```
crop_size = (320, 480)
voc_train = VOCSegDataset(True, crop_size, voc_dir)
voc_test = VOCSegDataset(False, crop_size, voc_dir)
```

```
read 1114 examples
read 1078 examples
```

We set the batch size to 64 and define the iterators for the training and testing sets. Print the shape of the first mini-batch. In contrast to image classification and object recognition, labels here are three-dimensional arrays.

```
batch_size = 64
train_iter = gluon.data.DataLoader(voc_train, batch_size, shuffle=True,
                                   last_batch='discard',
                                   num_workers=d2l.get_dataloader_workers())
for X, Y in train_iter:
    print(X.shape)
    print(Y.shape)
    break
```

```
(64, 3, 320, 480)
(64, 320, 480)
```

### 14.9.3 Put All Things Together

Finally, we define a function `load_data_voc` that downloads and loads this data set, and then returns the data loaders.

```
# Save to the d2l package.
def load_data_voc(batch_size, crop_size):
    """Download and load the VOC2012 semantic dataset."""
    voc_dir = d2l.download_voc_pascal()
    num_workers = d2l.get_dataloader_workers()
    train_iter = gluon.data.DataLoader(
        VOCSegDataset(True, crop_size, voc_dir), batch_size,
        shuffle=True, last_batch='discard', num_workers=num_workers)
    test_iter = gluon.data.DataLoader(
        VOCSegDataset(False, crop_size, voc_dir), batch_size,
        last_batch='discard', num_workers=num_workers)
    return train_iter, test_iter
```

### 14.9.4 Summary

- Semantic segmentation looks at how images can be segmented into regions with different semantic categories.

- In the semantic segmentation field, one important data set is Pascal VOC2012.
- Because the input images and labels in semantic segmentation have a one-to-one correspondence at the pixel level, we randomly crop them to a fixed size, rather than scaling them.

### 14.9.5 Exercises

- Recall the content we covered in Section 14.1. Which of the image augmentation methods used in image classification would be hard to use in semantic segmentation?

### 14.9.6 Scan the QR Code to Discuss<sup>189</sup>



## 14.10 Transposed Convolution

The layers we introduced so far for convolutional neural networks, including convolutional layers (Section 8.2) and pooling layers (Section 8.5), often reduce the input width and height, or keep them unchanged. Applications such as semantic segmentation (Section 14.9) and generative adversarial networks (Section 16.2), however, require to predict values for each pixel and therefore needs to increase input width and height. Transposed convolution, also named fractionally-strided convolution Dumoulin.Visin.2016 or deconvolution Long.Shelhamer.Darrell.2015, serves this purpose.

```
from mxnet import nd, init
from mxnet.gluon import nn
import d2l
```

### 14.10.1 Basic 2D Transposed Convolution

Let's consider a basic case that both input and output channels are 1, with 0 padding and 1 stride. Fig. 14.10.1 illustrates how transposed convolution with a  $2 \times 2$  kernel is computed on the  $2 \times 2$  input matrix.

Input	Kernel		Output
$\begin{matrix} 0 & 1 \\ 2 & 3 \end{matrix}$	$\begin{matrix} 0 & 1 \\ 2 & 3 \end{matrix}$	$=$	$\begin{matrix} 0 & 0 & \cdot \\ 0 & 0 & \cdot \\ \cdot & \cdot & \cdot \end{matrix}$
		$+$	$\begin{matrix} \cdot & 0 & 1 \\ \cdot & 2 & 3 \end{matrix}$
		$+$	$\begin{matrix} \cdot & \cdot & \cdot \\ 0 & 2 & \cdot \\ \cdot & \cdot & \cdot \end{matrix}$
		$+$	$\begin{matrix} \cdot & \cdot & \cdot \\ \cdot & 0 & 3 \\ \cdot & 6 & \cdot \end{matrix}$
		$=$	$\begin{matrix} 0 & 0 & 1 \\ 0 & 4 & 6 \\ 4 & 12 & 9 \end{matrix}$

Fig. 14.10.1: Transposed convolution layer with a  $2 \times 2$  kernel.

We can implement this operation by giving matrix kernel  $K$  and matrix input  $X$ .

<sup>189</sup> <https://discuss.mxnet.io/t/2448>

```
def trans_conv(X, K):
    h, w = K.shape
    Y = nd.zeros((X.shape[0] + h - 1, X.shape[1] + w - 1))
    for i in range(X.shape[0]):
        for j in range(X.shape[1]):
            Y[i: i + h, j: j + w] += X[i, j] * K
    return Y
```

Remember the convolution computes results by  $Y[i, j] = (X[i: i + h, j: j + w] * K).sum()$  (refer to `corr2d` in Section 8.2), which summarizes input values through the kernel. While the transposed convolution broadcasts input values through the kernel, which results in a larger output shape.

Verify the results in Fig. 14.10.1.

```
X = nd.array([[0,1], [2,3]])
K = nd.array([[0,1], [2,3]])
trans_conv(X, K)
```

```
[[ 0.  0.  1.]
 [ 0.  4.  6.]
 [ 4. 12.  9.]]
<NDArray 3x3 @cpu(0)>
```

Or we can use `nn.Conv2DTranspose` to obtain the same results. As `nn.Conv2D`, both input and kernel should be 4-D tensors.

```
X, K = X.reshape((1, 1, 2, 2)), K.reshape((1, 1, 2, 2))
tconv = nn.Conv2DTranspose(1, kernel_size=2)
tconv.initialize(init.Constant(K))
tconv(X)
```

```
[[[[ 0.  0.  1.]
   [ 0.  4.  6.]
   [ 4. 12.  9.]]]]
<NDArray 1x1x3x3 @cpu(0)>
```

## 14.10.2 Padding, Strides, and Channels

We apply padding elements to the input in convolution, while they are applied to the output in transposed convolution. A  $1 \times 1$  padding means we first compute the output as normal, then remove the first/last rows and columns.

```
tconv = nn.Conv2DTranspose(1, kernel_size=2, padding=1)
tconv.initialize(init.Constant(K))
tconv(X)
```

```
[[[[4.]]]]
<NDArray 1x1x1x1 @cpu(0)>
```

Similarly, strides are applied to outputs as well.

```
tconv = nn.Conv2DTranspose(1, kernel_size=2, strides=2)
tconv.initialize(init.Constant(K))
tconv(X)
```

```
[[[0. 0. 0. 1.]
 [0. 0. 2. 3.]
 [0. 2. 0. 3.]
 [4. 6. 6. 9.]]]
<NDArray 1x1x4x4 @cpu(0)>
```

The multi-channel extension of the transposed convolution is the same as the convolution. When the input has multiple channels, denoted by  $c_i$ , the transposed convolution assigns a  $k_h \times k_w$  kernel matrix to each input channel. If the output has a channel size  $c_o$ , then we have a  $c_i \times k_h \times k_w$  kernel for each output channel.

As a result, if we feed  $X$  into a convolutional layer  $f$  to compute  $Y = f(X)$  and create a transposed convolution layer  $g$  with the same hyper-parameters as  $f$  except for the output channel set to be the channel size of  $X$ , then  $g(Y)$  should have the same shape as  $X$ . Let's verify this statement.

```
X = nd.random.uniform(shape=(1, 10, 16, 16))
conv = nn.Conv2D(20, kernel_size=5, padding=2, strides=3)
tconv = nn.Conv2DTranspose(10, kernel_size=5, padding=2, strides=3)
conv.initialize()
tconv.initialize()
tconv(conv(X)).shape == X.shape
```

```
True
```

### 14.10.3 Analogy to Matrix Transposition

The transposed convolution takes its name from the matrix transposition. In fact, convolution operations can also be achieved by matrix multiplication. In the example below, we define a  $3 \times$  input  $X$  with a  $2 \times 2$  kernel  $K$ , and then use `corr2d` to compute the convolution output.

```
X = nd.arange(9).reshape((3,3))
K = nd.array([[0,1], [2,3]])
Y = d2l.corr2d(X, K)
Y
```

```
[[19. 25.]
 [37. 43.]]
<NDArray 2x2 @cpu(0)>
```

Next, we rewrite convolution kernel  $K$  as a matrix  $W$ . Its shape will be  $(4, 9)$ , where the  $i$ -th row present applying the kernel to the input to generate the  $i$ -th output element.

```
def kernel2matrix(K):
    k, W = nd.zeros(5), nd.zeros((4, 9))
    k[:2], k[3:5] = K[0,:], K[1,:]
    W[0, :5], W[1, 1:6], W[2, 3:8], W[3, 4:] = k, k, k, k
    return W
```

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```
W = kernel2matrix(K)
W
```

```
[[0. 1. 0. 2. 3. 0. 0. 0. 0.]
 [0. 0. 1. 0. 2. 3. 0. 0. 0.]
 [0. 0. 0. 0. 1. 0. 2. 3. 0.]
 [0. 0. 0. 0. 0. 1. 0. 2. 3.]]
<NDArray 4x9 @cpu(0)>
```

Then the convolution operator can be implemented by matrix multiplication with proper reshaping.

```
Y == nd.dot(W, X.reshape((-1)).reshape((2,2))
```

```
[[1. 1.]
 [1. 1.]]
<NDArray 2x2 @cpu(0)>
```

We can implement transposed convolution as a matrix multiplication as well by reusing `kernel2matrix`. To reuse the generated  $W$ , we construct a  $2 \times 2$  input, so the corresponding weight matrix will have a shape  $(9, 4)$ , which is  $W^T$ . Let's verify the results.

```
X = nd.array([[0,1], [2,3]])
Y = trans_conv(X, K)
Y == nd.dot(W.T, X.reshape((-1)).reshape((3,3))
```

```
[[1. 1. 1.]
 [1. 1. 1.]
 [1. 1. 1.]]
<NDArray 3x3 @cpu(0)>
```

#### 14.10.4 Summary

- Compared to convolutions that reduce inputs through kernels, transposed convolutions broadcast inputs.
- If a convolution layer reduces the input width and height by  $n_w$  and  $n_h$  time, respectively. Then a transposed convolution layer with the same kernel sizes, padding and strides will increase the input width and height by  $n_w$  and  $n_h$ , respectively.
- We can implement convolution operations by the matrix multiplication, the corresponding transposed convolutions can be done by transposed matrix multiplication.

#### 14.10.5 Exercises

- Is it efficient to use matrix multiplication to implement convolution operations? Why?

### 14.11 Fully Convolutional Networks (FCN)

We previously discussed semantic segmentation using each pixel in an image for category prediction. A fully convolutional network (FCN) Long.Shelhamer.Darrell.2015 uses a convolutional neural network to transform

image pixels to pixel categories. Unlike the convolutional neural networks previously introduced, an FCN transforms the height and width of the intermediate layer feature map back to the size of input image through the transposed convolution layer, so that the predictions have a one-to-one correspondence with input image in spatial dimension (height and width). Given a position on the spatial dimension, the output of the channel dimension will be a category prediction of the pixel corresponding to the location.

We will first import the package or module needed for the experiment and then explain the transposed convolution layer.

```
%matplotlib inline
import d2l
from mxnet import gluon, image, init, nd
from mxnet.gluon import nn
import numpy as np
```

### 14.11.1 Construct a Model

Here, we demonstrate the most basic design of a fully convolutional network model. As shown in Fig. 14.11.1, the fully convolutional network first uses the convolutional neural network to extract image features, then transforms the number of channels into the number of categories through the  $1 \times 1$  convolution layer, and finally transforms the height and width of the feature map to the size of the input image by using the transposed convolution layer Section 14.10. The model output has the same height and width as the input image and has a one-to-one correspondence in spatial positions. The final output channel contains the category prediction of the pixel of the corresponding spatial position.

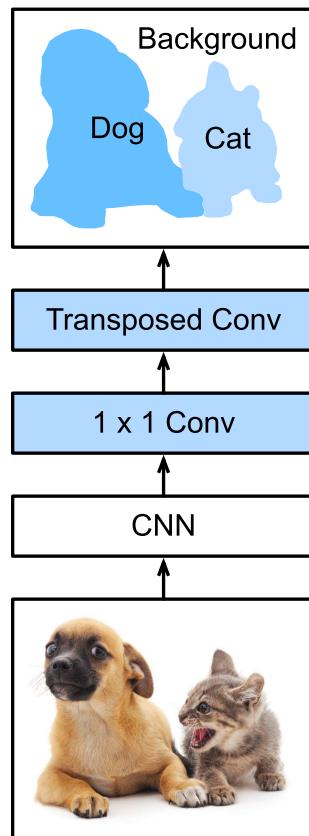


Fig. 14.11.1: Fully convolutional network.

Below, we use a ResNet-18 model pre-trained on the ImageNet data set to extract image features and record the network instance as `pretrained_net`. As you can see, the last two layers of the model member variable `features` are the global maximum pooling layer `GlobalAvgPool2D` and example flattening layer `Flatten`. The `output` module contains the fully connected layer used for output. These layers are not required for a fully convolutional network.

```
pretrained_net = gluon.model_zoo.vision.resnet18_v2(pretrained=True)
pretrained_net.features[-4:], pretrained_net.output

(HybridSequential(
    (0): BatchNorm(axis=1, eps=1e-05, momentum=0.9, fix_gamma=False, use_global_
     ↲ stats=False, in_channels=512)
    (1): Activation(relu)
    (2): GlobalAvgPool2D(size=(1, 1), stride=(1, 1), padding=(0, 0), ceil_mode=True)
    (3): Flatten
), Dense(512 -> 1000, linear))
```

Next, we create the fully convolutional network instance `net`. It duplicates all the neural layers except the last two layers of the instance member variable `features` of `pretrained_net` and the model parameters obtained after pre-training.

```
net = nn.HybridSequential()
for layer in pretrained_net.features[:-2]:
    net.add(layer)
```

Given an input of a height and width of 320 and 480 respectively, the forward computation of `net` will reduce the height and width of the input to 1/32 of the original, i.e. 10 and 15.

```
X = nd.random.uniform(shape=(1, 3, 320, 480))
net(X).shape
```

```
(1, 512, 10, 15)
```

Next, we transform the number of output channels to the number of categories Pascal VOC2012 (21) through the  $1 \times 1$  convolution layer. Finally, we need to magnify the height and width of the feature map by a factor of 32 to change them back to the height and width of the input image. Recall the calculation method for the convolution layer output shape described in Section 8.3. Because  $(320 - 64 + 16 \times 2 + 32)/32 = 10$  and  $(480 - 64 + 16 \times 2 + 32)/32 = 15$ , we construct a transposed convolution layer with a stride of 32 and set the height and width of the convolution kernel to 64 and the padding to 16. It is not difficult to see that, if the stride is  $s$ , the padding is  $s/2$  (assuming  $s/2$  is an integer), and the height and width of the convolution kernel are  $2s$ , the transposed convolution kernel will magnify both the height and width of the input by a factor of  $s$ .

```
num_classes = 21
net.add(nn.Conv2D(num_classes, kernel_size=1,
                 nn.Conv2DTranspose(
                     num_classes, kernel_size=64, padding=16, strides=32))
```

### 14.11.2 Initialize the Transposed Convolution Layer

We already know that the transposed convolution layer can magnify a feature map. In image processing, sometimes we need to magnify the image, i.e. upsampling. There are many methods for upsampling, and one common method is bilinear interpolation. Simply speaking, in order to get the pixel of the output image at

the coordinates  $(x, y)$ , the coordinates are first mapped to the coordinates of the input image  $(x', y')$ . This can be done based on the ratio of the size of the input to the size of the output. The mapped values  $x'$  and  $y'$  are usually real numbers. Then, we find the four pixels closest to the coordinate  $(x', y')$  on the input image. Finally, the pixels of the output image at coordinates  $(x, y)$  are calculated based on these four pixels on the input image and their relative distances to  $(x', y')$ . Upsampling by bilinear interpolation can be implemented by transposed convolution layer of the convolution kernel constructed using the following `bilinear_kernel` function. Due to space limitations, we only give the implementation of the `bilinear_kernel` function and will not discuss the principles of the algorithm.

```
def bilinear_kernel(in_channels, out_channels, kernel_size):
    factor = (kernel_size + 1) // 2
    if kernel_size % 2 == 1:
        center = factor - 1
    else:
        center = factor - 0.5
    og = np.ogrid[:kernel_size, :kernel_size]
    filt = (1 - abs(og[0] - center) / factor) * \
           (1 - abs(og[1] - center) / factor)
    weight = np.zeros((in_channels, out_channels, kernel_size, kernel_size),
                      dtype='float32')
    weight[:, :, :, range(out_channels)] = filt
    return nd.array(weight)
```

Now, we will experiment with bilinear interpolation upsampling implemented by transposed convolution layers. Construct a transposed convolution layer that magnifies height and width of input by a factor of 2 and initialize its convolution kernel with the `bilinear_kernel` function.

```
conv_trans = nn.Conv2DTranspose(3, kernel_size=4, padding=1, strides=2)
conv_trans.initialize(init.Constant(bilinear_kernel(3, 3, 4)))
```

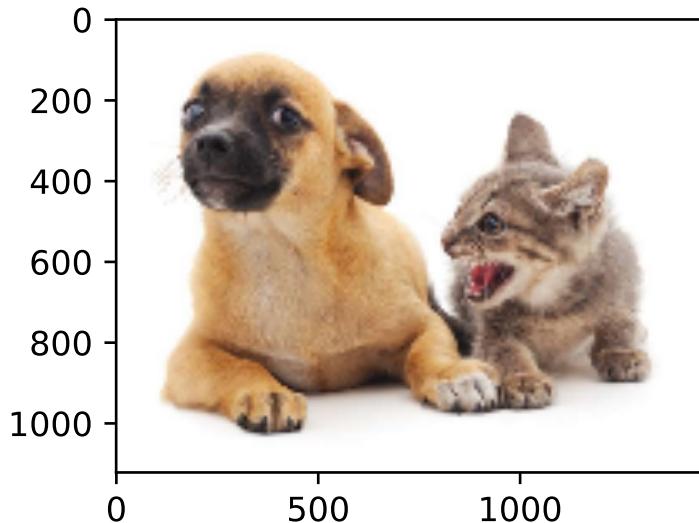
Read the image `X` and record the result of upsampling as `Y`. In order to print the image, we need to adjust the position of the channel dimension.

```
img = image.imread('../img/catdog.jpg')
X = img.astype('float32').transpose((2, 0, 1)).expand_dims(axis=0) / 255
Y = conv_trans(X)
out_img = Y[0].transpose((1, 2, 0))
```

As you can see, the transposed convolution layer magnifies both the height and width of the image by a factor of 2. It is worth mentioning that, besides to the difference in coordinate scale, the image magnified by bilinear interpolation and original image printed in [Section 14.3](#) look the same.

```
d2l.set_figsize((3.5, 2.5))
print('input image shape:', img.shape)
d2l.plt.imshow(img.asnumpy());
print('output image shape:', out_img.shape)
d2l.plt.imshow(out_img.asnumpy());
```

```
input image shape: (561, 728, 3)
output image shape: (1122, 1456, 3)
```



In a fully convolutional network, we initialize the transposed convolution layer for upsampled bilinear interpolation. For a  $1 \times 1$  convolution layer, we use Xavier for randomly initialization.

```
W = bilinear_kernel(num_classes, num_classes, 64)
net[-1].initialize(init.Constant(W))
net[-2].initialize(init=init.Xavier())
```

### 14.11.3 Read the Data Set

We read the data set using the method described in the previous section. Here, we specify shape of the randomly cropped output image as  $320 \times 480$ , so both the height and width are divisible by 32.

```
batch_size, crop_size = 32, (320, 480)
train_iter, test_iter = d2l.load_data_voc(batch_size, crop_size)
```

```
Downloading ../data/VOCtrainval_11-May-2012.tar from http://data.mxnet.io/data/
→ VOCtrainval_11-May-2012.tar...
read 1114 examples
read 1078 examples
```

### 14.11.4 Training

Now we can start training the model. The loss function and accuracy calculation here are not substantially different from those used in image classification. Because we use the channel of the transposed convolution layer to predict pixel categories, the `axis=1` (channel dimension) option is specified in `SoftmaxCrossEntropyLoss`. In addition, the model calculates the accuracy based on whether the prediction category of each pixel is correct.

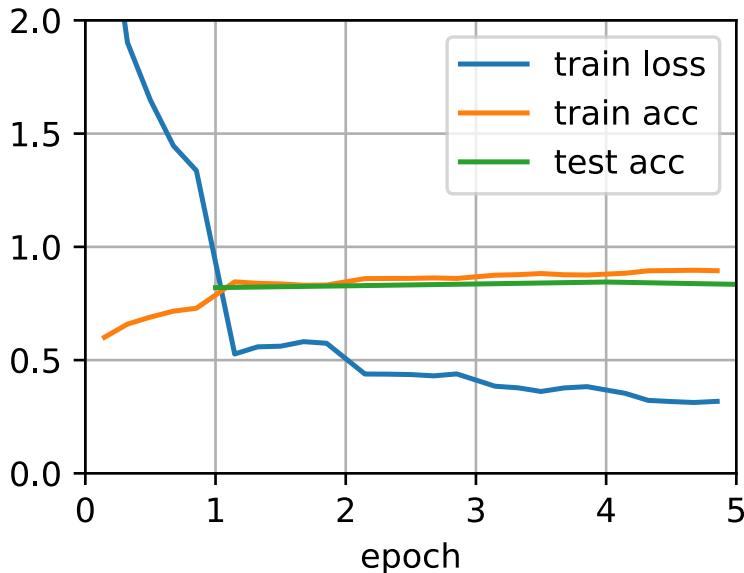
```
num_epochs, lr, wd, ctx = 5, 0.1, 1e-3, d2l.try_all_gpus()
loss = gluon.loss.SoftmaxCrossEntropyLoss(axis=1)
net.collect_params().reset_ctx(ctx)
trainer = gluon.Trainer(net.collect_params(), 'sgd',
```

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```
{'learning_rate': lr, 'wd': wd})
d2l.train_ch12(net, train_iter, test_iter, loss, trainer, num_epochs, ctx)
```

```
loss 0.323, train acc 0.893, test acc 0.834
286.4 examples/sec on [gpu(0), gpu(1)]
```



### 14.11.5 Prediction

During predicting, we need to standardize the input image in each channel and transform them into the four-dimensional input format required by the convolutional neural network.

```
def predict(img):
    X = test_iter._dataset.normalize_image(img)
    X = X.transpose((2, 0, 1)).expand_dims(axis=0)
    pred = nd.argmax(net(X.as_in_context(ctx[0])), axis=1)
    return pred.reshape((pred.shape[1], pred.shape[2]))
```

To visualize the predicted categories for each pixel, we map the predicted categories back to their labeled colors in the data set.

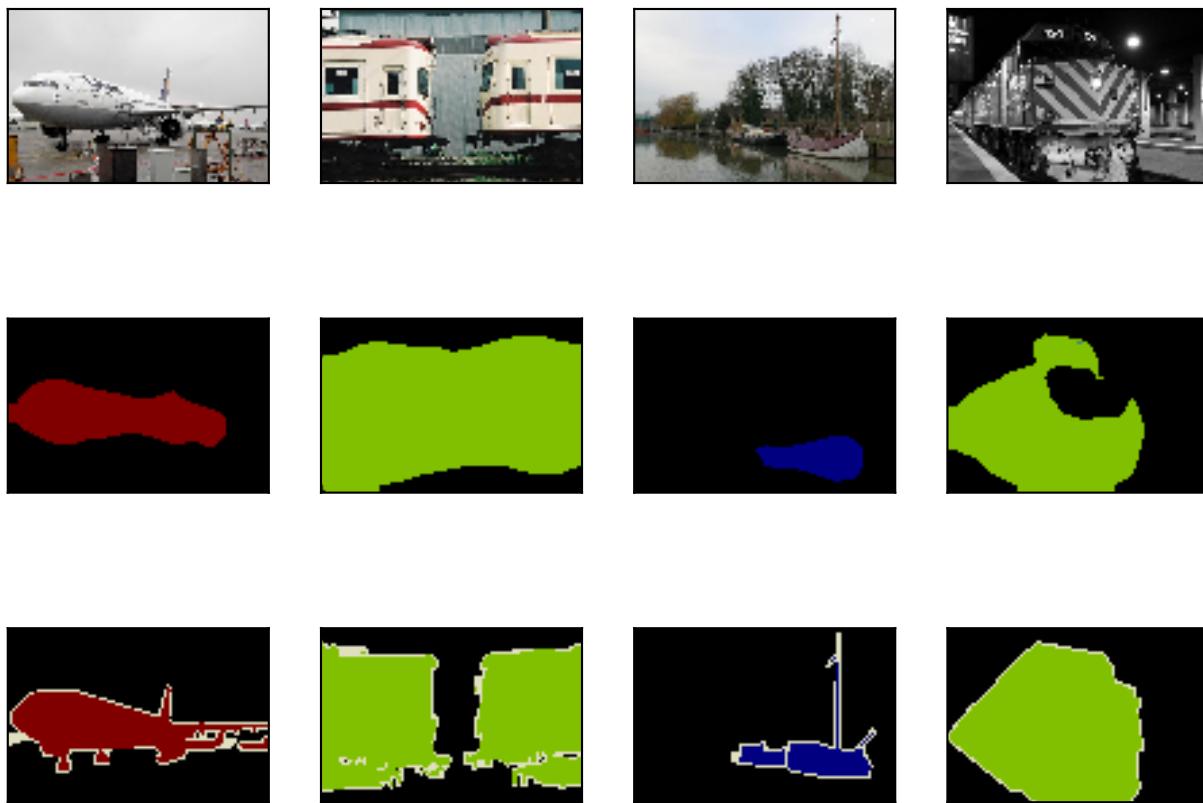
```
def label2image(pred):
    colormap = nd.array(d2l.VOC_COLORMAP, ctx=ctx[0], dtype='uint8')
    X = pred.astype('int32')
    return colormap[X, :]
```

The size and shape of the images in the test data set vary. Because the model uses a transposed convolution layer with a stride of 32, when the height or width of the input image is not divisible by 32, the height or width of the transposed convolution layer output deviates from the size of the input image. In order to solve this problem, we can crop multiple rectangular areas in the image with heights and widths as integer multiples of 32, and then perform forward computation on the pixels in these areas. When combined, these areas must completely cover the input image. When a pixel is covered by multiple areas, the average of the

transposed convolution layer output in the forward computation of the different areas can be used as an input for the softmax operation to predict the category.

For the sake of simplicity, we only read a few large test images and crop an area with a shape of  $320 \times 480$  from the top-left corner of the image. Only this area is used for prediction. For the input image, we print the cropped area first, then print the predicted result, and finally print the labeled category.

```
test_images, test_labels = d2l.read_voc_images(is_train=False)
n, imgs = 4, []
for i in range(n):
    crop_rect = (0, 0, 480, 320)
    X = image.fixed_crop(test_images[i], *crop_rect)
    pred = label2image(predict(X))
    imgs += [X, pred, image.fixed_crop(test_labels[i], *crop_rect)]
d2l.show_images(imgs[::3] + imgs[1::3] + imgs[2::3], 3, n, scale=2);
```



### 14.11.6 Summary

- The fully convolutional network first uses the convolutional neural network to extract image features, then transforms the number of channels into the number of categories through the  $1 \times 1$  convolution layer, and finally transforms the height and width of the feature map to the size of the input image by using the transposed convolution layer to output the category of each pixel.
- In a fully convolutional network, we initialize the transposed convolution layer for upsampled bilinear interpolation.

### 14.11.7 Exercises

- If we use Xavier to randomly initialize the transposed convolution layer, what will happen to the result?
- Can you further improve the accuracy of the model by tuning the hyper-parameters?
- Predict the categories of all pixels in the test image.
- The outputs of some intermediate layers of the convolutional neural network are also used in the paper on fully convolutional networks[1]. Try to implement this idea.

### 14.11.8 Scan the QR Code to Discuss<sup>190</sup>



## 14.12 Neural Style Transfer

If you use social sharing apps or happen to be an amateur photographer, you are familiar with filters. Filters can alter the color styles of photos to make the background sharper or people's faces whiter. However, a filter generally can only change one aspect of a photo. To create the ideal photo, you often need to try many different filter combinations. This process is as complex as tuning the hyper-parameters of a model.

In this section, we will discuss how we can use convolution neural networks (CNNs) to automatically apply the style of one image to another image, an operation known as style transfer [15]. Here, we need two input images, one content image and one style image. We use a neural network to alter the content image so that its style mirrors that of the style image. In Fig. 14.12.1, the content image is a landscape photo the author took in Mount Rainier National Park near Seattle. The style image is an oil painting of oak trees in autumn. The output composite image retains the overall shapes of the objects in the content image, but applies the oil painting brushwork of the style image and makes the overall color more vivid.

### 14.12.1 Technique

The CNN-based style transfer model is shown in Fig. 14.12.2. First, we initialize the composite image. For example, we can initialize it as the content image. This composite image is the only variable that needs to be updated in the style transfer process, i.e. the model parameter to be updated in style transfer. Then, we select a pre-trained CNN to extract image features. These model parameters do not need to be updated during training. The deep CNN uses multiple neural layers that successively extract image features. We can select the output of certain layers to use as content features or style features. If we use the structure in Fig. 14.12.2, the pretrained neural network contains three convolutional layers. The second layer outputs the image content features, while the outputs of the first and third layers are used as style features. Next, we use forward propagation (in the direction of the solid lines) to compute the style transfer loss function and backward propagation (in the direction of the dotted lines) to update the model parameter, constantly updating the composite image. The loss functions used in style transfer generally have three parts: 1. Content loss is used to make the composite image approximate the content image as regards content features. 2. Style loss is used to make the composite image approximate the style image in terms of style features. 3. Total

<sup>190</sup> <https://discuss.mxnet.io/t/2454>

Content image



Composite image



Style image



Fig. 14.12.1: Content and style input images and composite image produced by style transfer.

variation loss helps reduce the noise in the composite image. Finally, after we finish training the model, we output the style transfer model parameters to obtain the final composite image.

Next, we will perform an experiment to help us better understand the technical details of style transfer.

### 14.12.2 Read the Content and Style Images

First, we read the content and style images. By printing out the image coordinate axes, we can see that they have different dimensions.

```
%matplotlib inline
import d2l
from mxnet import autograd, gluon, image, init, nd
from mxnet.gluon import nn

d2l.set_figsize((3.5, 2.5))
content_img = image.imread('../img/rainier.jpg')
d2l.plt.imshow(content_img.asnumpy());
```

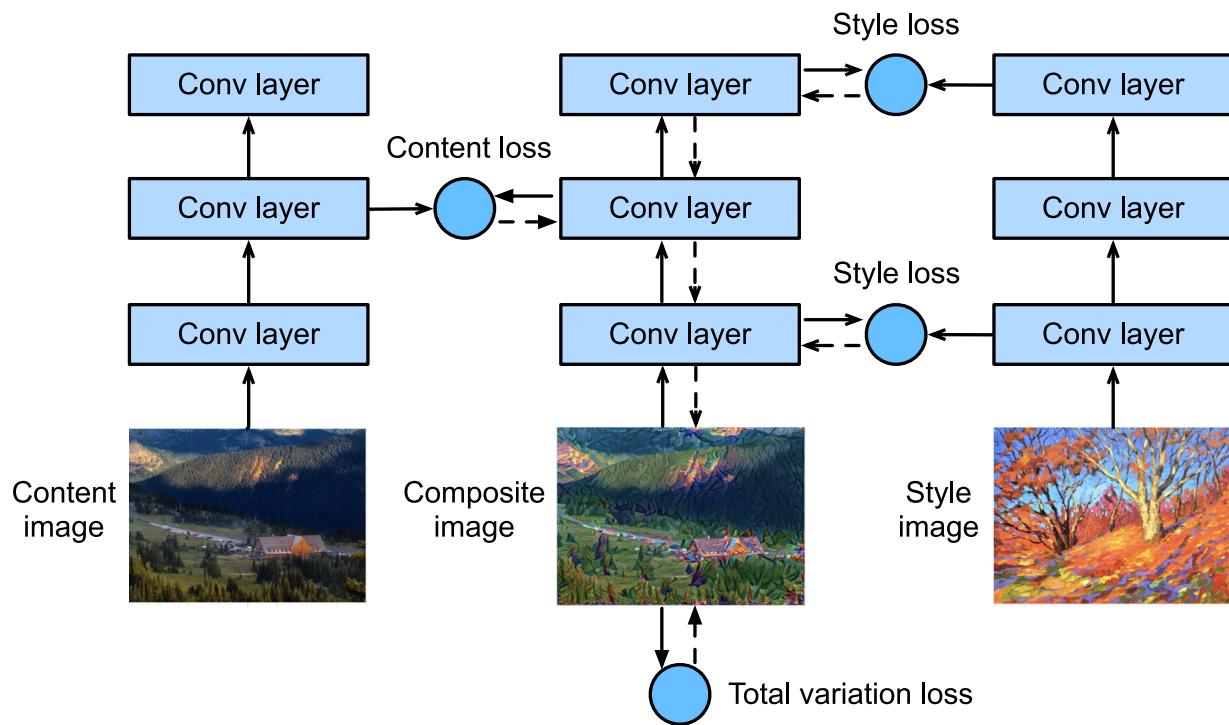
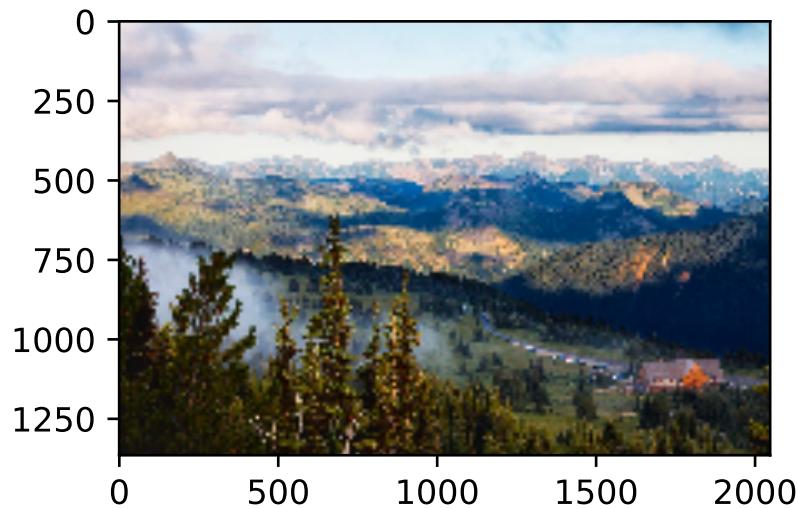
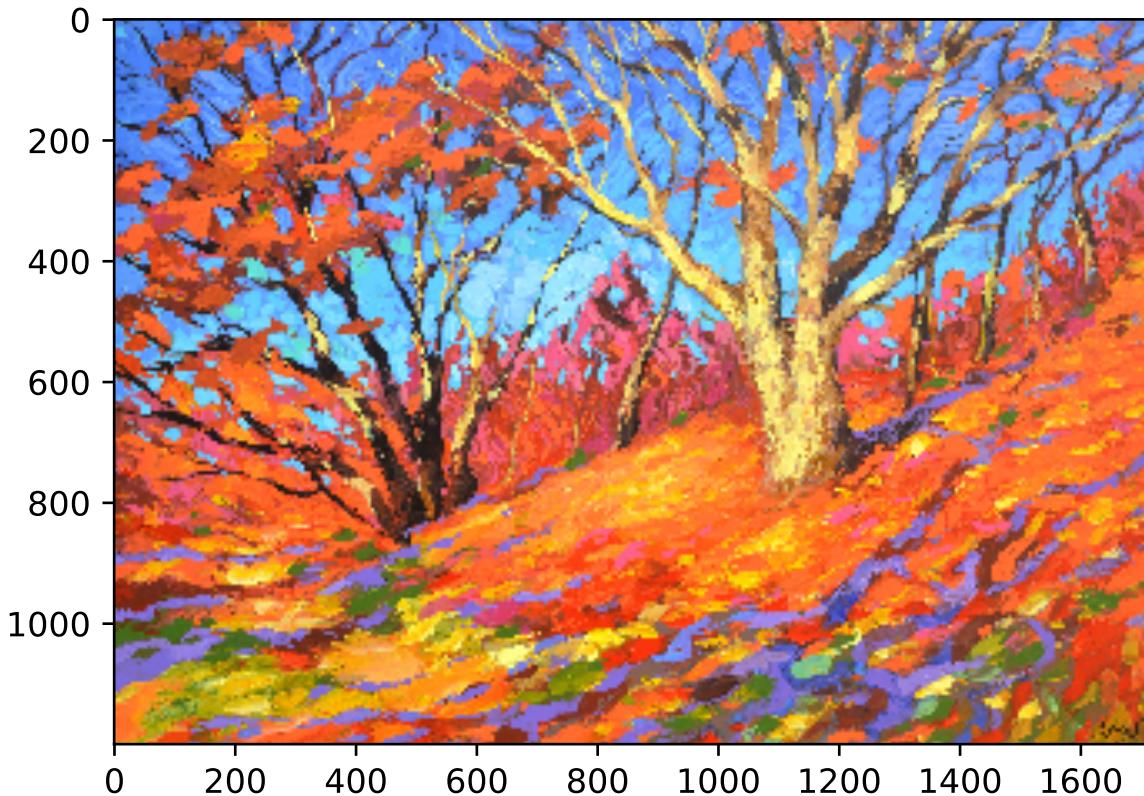


Fig. 14.12.2: CNN-based style transfer process. Solid lines show the direction of forward propagation and dotted lines show backward propagation.



```
style_img = image.imread('../img/autumn_oak.jpg')
d2l.plt.imshow(style_img.asnumpy());
```



### 14.12.3 Preprocessing and Postprocessing

Below, we define the functions for image preprocessing and postprocessing. The `preprocess` function normalizes each of the three RGB channels of the input images and transforms the results to a format that can be input to the CNN. The `postprocess` function restores the pixel values in the output image to their original values before normalization. Because the image printing function requires that each pixel has a floating point value from 0 to 1, we use the `clip` function to replace values smaller than 0 or greater than 1 with 0 or 1, respectively.

```
rgb_mean = nd.array([0.485, 0.456, 0.406])
rgb_std = nd.array([0.229, 0.224, 0.225])

def preprocess(img, image_shape):
    img = img.imresize(*image_shape)
    img = (img.astype('float32') / 255 - rgb_mean) / rgb_std
    return img.transpose((2, 0, 1)).expand_dims(axis=0)

def postprocess(img):
    img = img[0].as_in_context(rgb_std.context)
    return (img.transpose((1, 2, 0)) * rgb_std + rgb_mean).clip(0, 1)
```

### 14.12.4 Extract Features

We use the VGG-19 model pre-trained on the ImageNet data set to extract image features[1].

```
pretrained_net = gluon.model_zoo.vision.vgg19(pretrained=True)
```

To extract image content and style features, we can select the outputs of certain layers in the VGG network. In general, the closer an output is to the input layer, the easier it is to extract image detail information. The farther away an output is, the easier it is to extract global information. To prevent the composite image from retaining too many details from the content image, we select a VGG network layer near the output layer to output the image content features. This layer is called the content layer. We also select the outputs of different layers from the VGG network for matching local and global styles. These are called the style layers. As we mentioned in [Section 9.2](#), VGG networks have five convolutional blocks. In this experiment, we select the last convolutional layer of the fourth convolutional block as the content layer and the first layer of each block as style layers. We can obtain the indexes for these layers by printing the `pretrained_net` instance.

```
style_layers, content_layers = [0, 5, 10, 19, 28], [25]
```

During feature extraction, we only need to use all the VGG layers from the input layer to the content or style layer nearest the output layer. Below, we build a new network, `net`, which only retains the layers in the VGG network we need to use. We then use `net` to extract features.

```
net = nn.Sequential()
for i in range(max(content_layers + style_layers) + 1):
    net.add(pretrained_net.features[i])
```

Given input `X`, if we simply call the forward computation `net(X)`, we can only obtain the output of the last layer. Because we also need the outputs of the intermediate layers, we need to perform layer-by-layer computation and retain the content and style layer outputs.

```
def extract_features(X, content_layers, style_layers):
    contents = []
    styles = []
    for i in range(len(net)):
        X = net[i](X)
        if i in style_layers:
            styles.append(X)
        if i in content_layers:
            contents.append(X)
    return contents, styles
```

Next, we define two functions: The `get_contents` function obtains the content features extracted from the content image, while the `get_styles` function obtains the style features extracted from the style image. Because we do not need to change the parameters of the pre-trained VGG model during training, we can extract the content features from the content image and style features from the style image before the start of training. As the composite image is the model parameter that must be updated during style transfer, we can only call the `extract_features` function during training to extract the content and style features of the composite image.

```
def get_contents(image_shape, ctx):
    content_X = preprocess(content_img, image_shape).copyto(ctx)
    contents_Y, _ = extract_features(content_X, content_layers, style_layers)
    return content_X, contents_Y

def get_styles(image_shape, ctx):
    style_X = preprocess(style_img, image_shape).copyto(ctx)
```

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```
_ , styles_Y = extract_features(style_X, content_layers, style_layers)
return style_X, styles_Y
```

### 14.12.5 Define the Loss Function

Next, we will look at the loss function used for style transfer. The loss function includes the content loss, style loss, and total variation loss.

#### Content Loss

Similar to the loss function used in linear regression, content loss uses a square error function to measure the difference in content features between the composite image and content image. The two inputs of the square error function are both content layer outputs obtained from the `extract_features` function.

```
def content_loss(Y_hat, Y):
    return (Y_hat - Y).square().mean()
```

#### Style Loss

Style loss, similar to content loss, uses a square error function to measure the difference in style between the composite image and style image. To express the styles output by the style layers, we first use the `extract_features` function to compute the style layer output. Assuming that the output has 1 example,  $c$  channels, and a height and width of  $h$  and  $w$ , we can transform the output into the matrix  $\mathbf{X}$ , which has  $c$  rows and  $h \cdot w$  columns. You can think of matrix  $\mathbf{X}$  as the combination of the  $c$  vectors  $\mathbf{x}_1, \dots, \mathbf{x}_c$ , which have a length of  $hw$ . Here, the vector  $\mathbf{x}_i$  represents the style feature of channel  $i$ . In the Gram matrix of these vectors  $\mathbf{X}\mathbf{X}^\top \in \mathbb{R}^{c \times c}$ , element  $x_{ij}$  in row  $i$  column  $j$  is the inner product of vectors  $\mathbf{x}_i$  and  $\mathbf{x}_j$ . It represents the correlation of the style features of channels  $i$  and  $j$ . We use this type of Gram matrix to represent the style output by the style layers. You must note that, when the  $h \cdot w$  value is large, this often leads to large values in the Gram matrix. In addition, the height and width of the Gram matrix are both the number of channels  $c$ . To ensure that the style loss is not affected by the size of these values, we define the `gram` function below to divide the Gram matrix by the number of its elements, i.e.  $c \cdot h \cdot w$ .

```
def gram(X):
    num_channels, n = X.shape[1], X.size // X.shape[1]
    X = X.reshape((num_channels, n))
    return nd.dot(X, X.T) / (num_channels * n)
```

Naturally, the two Gram matrix inputs of the square error function for style loss are taken from the composite image and style image style layer outputs. Here, we assume that the Gram matrix of the style image, `gram_Y`, has been computed in advance.

```
def style_loss(Y_hat, gram_Y):
    return (gram(Y_hat) - gram_Y).square().mean()
```

#### Total Variance Loss

Sometimes, the composite images we learn have a lot of high-frequency noise, particularly bright or dark pixels. One common noise reduction method is total variation denoising. We assume that  $x_{i,j}$  represents

the pixel value at the coordinate  $(i, j)$ , so the total variance loss is:

$$\sum_{i,j} |x_{i,j} - x_{i+1,j}| + |x_{i,j} - x_{i,j+1}| \quad (14.12.1)$$

We try to make the values of neighboring pixels as similar as possible.

```
def tv_loss(Y_hat):
    return 0.5 * ((Y_hat[:, :, 1:, :] - Y_hat[:, :, :-1, :]).abs().mean() +
                  (Y_hat[:, :, :, 1:] - Y_hat[:, :, :, :-1]).abs().mean())
```

### Loss Function

The loss function for style transfer is the weighted sum of the content loss, style loss, and total variance loss. By adjusting these weight hyper-parameters, we can balance the retained content, transferred style, and noise reduction in the composite image according to their relative importance.

```
content_weight, style_weight, tv_weight = 1, 1e3, 10

def compute_loss(X, contents_Y_hat, styles_Y_hat, contents_Y, styles_Y_gram):
    # Calculate the content, style, and total variance losses respectively
    contents_l = [content_loss(Y_hat, Y) * content_weight for Y_hat, Y in zip(
        contents_Y_hat, contents_Y)]
    styles_l = [style_loss(Y_hat, Y) * style_weight for Y_hat, Y in zip(
        styles_Y_hat, styles_Y_gram)]
    tv_l = tv_loss(X) * tv_weight
    # Add up all the losses
    l = nd.add_n(*styles_l) + nd.add_n(*contents_l) + tv_l
    return contents_l, styles_l, tv_l, l
```

### 14.12.6 Create and Initialize the Composite Image

In style transfer, the composite image is the only variable that needs to be updated. Therefore, we can define a simple model, `GeneratedImage`, and treat the composite image as a model parameter. In the model, forward computation only returns the model parameter.

```
class GeneratedImage(nn.Block):
    def __init__(self, img_shape, **kwargs):
        super(GeneratedImage, self).__init__(**kwargs)
        self.weight = self.params.get('weight', shape=img_shape)

    def forward(self):
        return self.weight.data()
```

Next, we define the `get_inits` function. This function creates a composite image model instance and initializes it to the image `X`. The Gram matrix for the various style layers of the style image, `styles_Y_gram`, is computed prior to training.

```
def get_inits(X, ctx, lr, styles_Y):
    gen_img = GeneratedImage(X.shape)
    gen_img.initialize(init.Constant(X), ctx=ctx, force_reinit=True)
    trainer = gluon.Trainer(gen_img.collect_params(), 'adam',
```

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```

        {'learning_rate': lr})
styles_Y_gram = [gram(Y) for Y in styles_Y]
return gen_img(), styles_Y_gram, trainer

```

### 14.12.7 Training

During model training, we constantly extract the content and style features of the composite image and calculate the loss function. Recall our discussion of how synchronization functions force the front end to wait for computation results in Section 13.2. Because we only call the `asscalar` synchronization function every 50 epochs, the process may occupy a great deal of memory. Therefore, we call the `waitall` synchronization function during every epoch.

```

def train(X, contents_Y, styles_Y, ctx, lr, num_epochs, lr_decay_epoch):
    X, styles_Y_gram, trainer = get_inits(X, ctx, lr, styles_Y)
    animator = d2l.Animator(xlabel='epoch', ylabel='loss', xlim=[1, num_epochs],
                            legend=['content', 'style', 'TV'],
                            ncols=2, figsize=(7, 2.5))
    for epoch in range(1, num_epochs+1):
        with autograd.record():
            contents_Y_hat, styles_Y_hat = extract_features(
                X, content_layers, style_layers)
            contents_l, styles_l, tv_l, l = compute_loss(
                X, contents_Y_hat, styles_Y_hat, contents_Y, styles_Y_gram)
            l.backward()
            trainer.step(1)
            nd.waitall()
            if epoch % lr_decay_epoch == 0:
                trainer.set_learning_rate(trainer.learning_rate * 0.1)
            if epoch % 10 == 0:
                animator.axes[1].imshow(postprocess(X).asnumpy())
                animator.add(epoch, [nd.add_n(*contents_l).asscalar(),
                                    nd.add_n(*styles_l).asscalar(), tv_l.asscalar()])
    return X

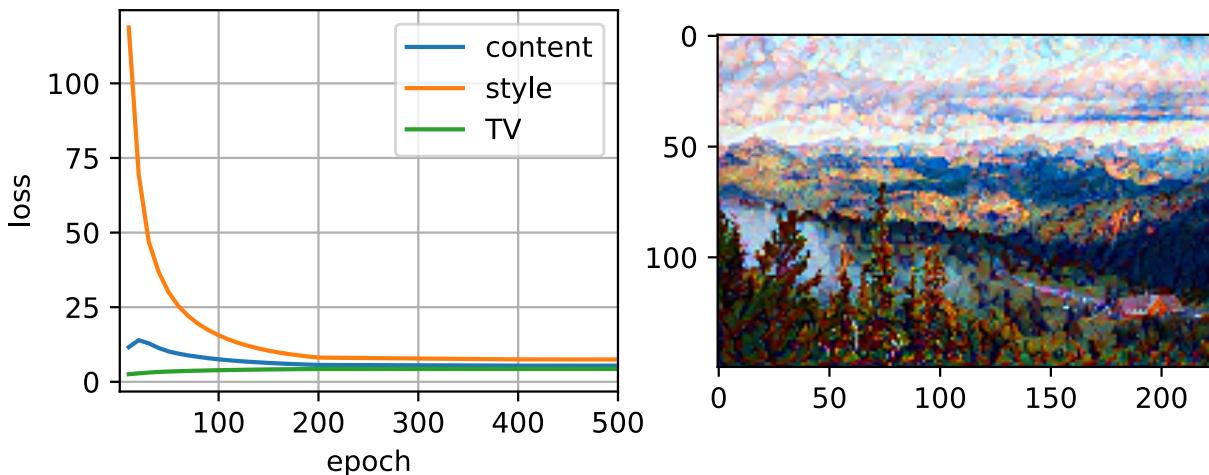
```

Next, we start to train the model. First, we set the height and width of the content and style images to 150 by 225 pixels. We use the content image to initialize the composite image.

```

ctx, image_shape = d2l.try_gpu(), (225, 150)
net.collect_params().reset_ctx(ctx)
content_X, contents_Y = get_contents(image_shape, ctx)
_, styles_Y = get_styles(image_shape, ctx)
output = train(content_X, contents_Y, styles_Y, ctx, 0.01, 500, 200)

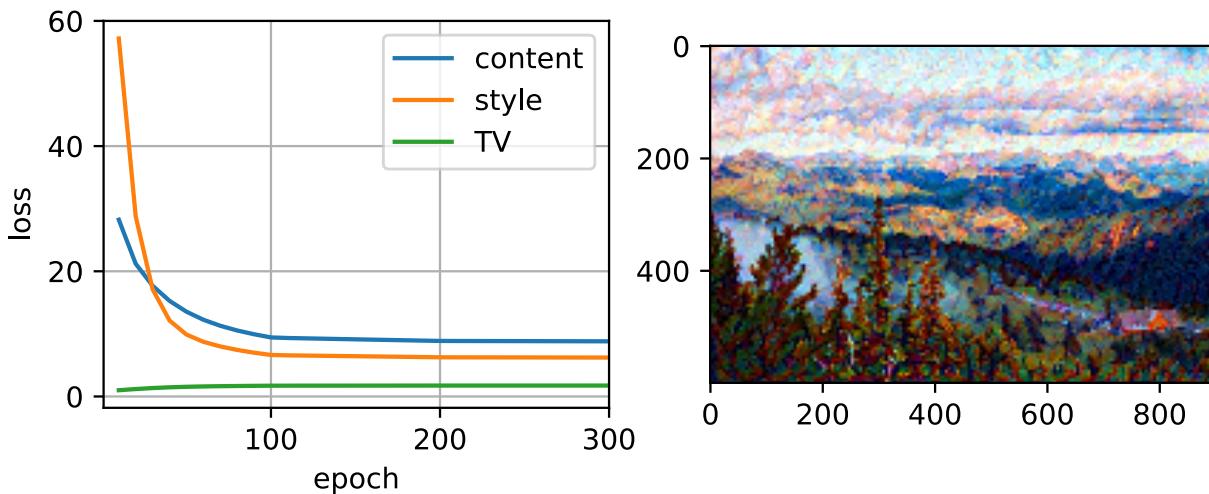
```



As you can see, the composite image retains the scenery and objects of the content image, while introducing the color of the style image. Because the image is relatively small, the details are a bit fuzzy.

To obtain a clearer composite image, we train the model using a larger image size:  $900 \times 600$ . We increase the height and width of the image used before by a factor of four and initialize a larger composite image.

```
image_shape = (900, 600)
_, content_Y = get_contents(image_shape, ctx)
_, style_Y = get_styles(image_shape, ctx)
X = preprocess(postprocess(output) * 255, image_shape)
output = train(X, content_Y, style_Y, ctx, 0.01, 300, 100)
d2l.plt.imwrite('../img/neural-style.png', postprocess(output).asnumpy())
```



As you can see, each epoch takes more time due to the larger image size. As shown in Fig. 14.12.3, the composite image produced retains more detail due to its larger size. The composite image not only has large blocks of color like the style image, but these blocks even have the subtle texture of brush strokes.

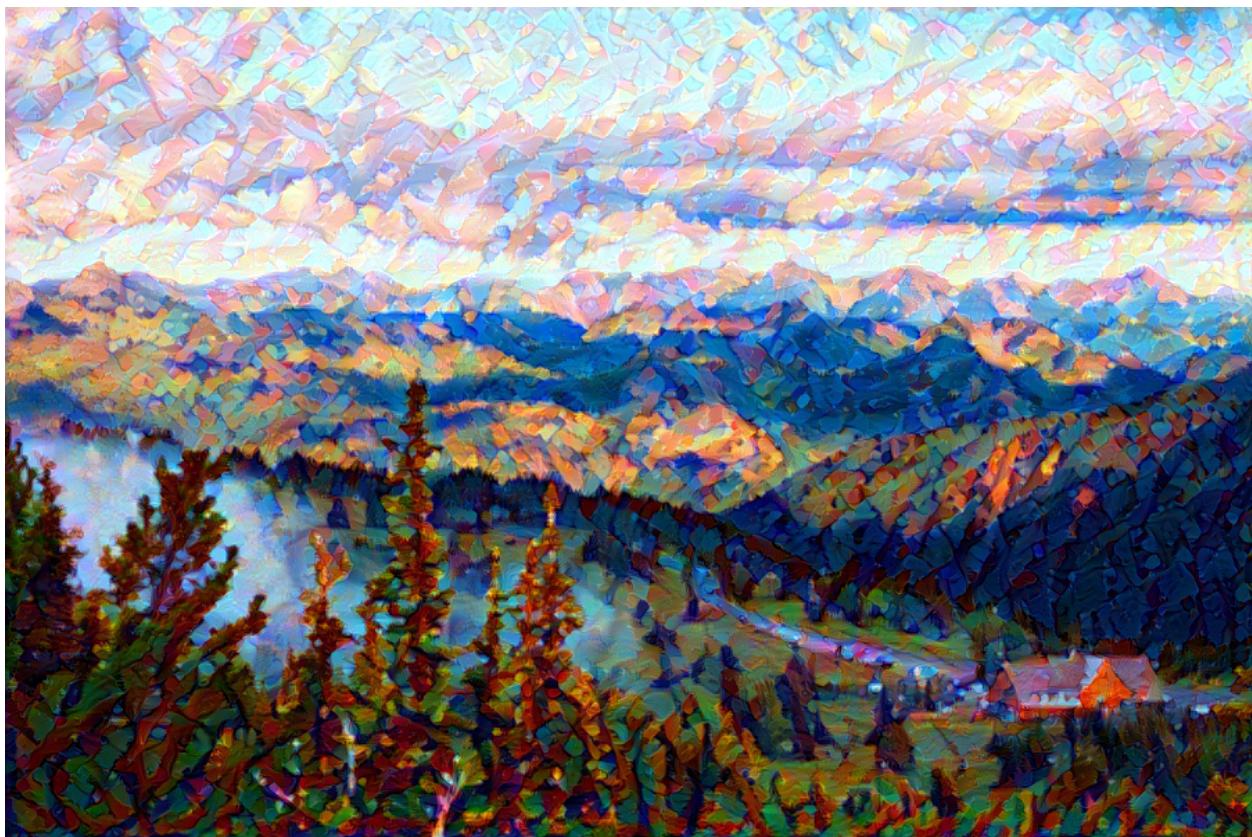


Fig. 14.12.3:  $900 \times 600$  composite image.

### 14.12.8 Summary

- The loss functions used in style transfer generally have three parts: 1. Content loss is used to make the composite image approximate the content image as regards content features. 2. Style loss is used to make the composite image approximate the style image in terms of style features. 3. Total variation loss helps reduce the noise in the composite image.
- We can use a pre-trained CNN to extract image features and minimize the loss function to continuously update the composite image.
- We use a Gram matrix to represent the style output by the style layers.

### 14.12.9 Exercises

- How does the output change when you select different content and style layers?
- Adjust the weight hyper-parameters in the loss function. Does the output retain more content or have less noise?
- Use different content and style images. Can you create more interesting composite images?

### 14.12.10 Scan the QR Code to Discuss<sup>191</sup>



## 14.13 Image Classification (CIFAR-10) on Kaggle

So far, we have been using Gluon's `data` package to directly obtain image data sets in `NDArray` format. In practice, however, image data sets often exist in the format of image files. In this section, we will start with the original image files and organize, read, and convert the files to `NDArray` format step by step.

We performed an experiment on the CIFAR-10 data set in Section 14.1. This is an important data set in the computer vision field. Now, we will apply the knowledge we learned in the previous sections in order to participate in the Kaggle competition, which addresses CIFAR-10 image classification problems. The competition's web address is

<https://www.kaggle.com/c/cifar-10>

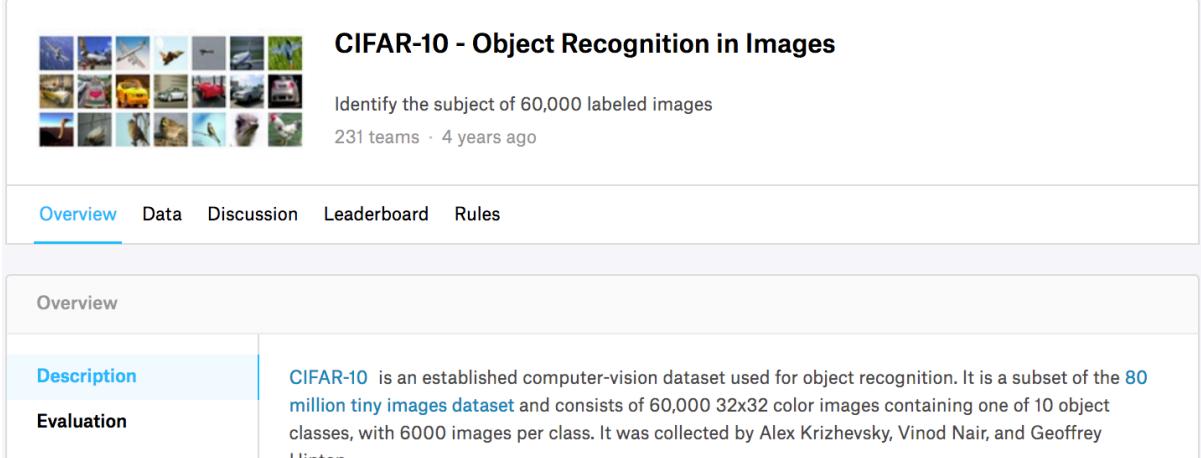
Figure 11.16 shows the information on the competition's webpage. In order to submit the results, please register an account on the Kaggle website first.

First, import the packages or modules required for the competition.

```
import d2l
from mxnet import autograd, gluon, init
from mxnet.gluon import nn
import os
```

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<sup>191</sup> <https://discuss.mxnet.io/t/2449>



The screenshot shows the Kaggle competition page for CIFAR-10. At the top, there's a grid of small sample images from the dataset. To the right of the images, the title "CIFAR-10 - Object Recognition in Images" is displayed. Below the title, it says "Identify the subject of 60,000 labeled images" and "231 teams · 4 years ago". A navigation bar below the title includes tabs for "Overview" (which is underlined in blue), "Data", "Discussion", "Leaderboard", and "Rules". The main content area has a header "Overview". On the left, there are two tabs: "Description" (selected) and "Evaluation". The "Description" tab contains text about the CIFAR-10 dataset, stating it's an established computer-vision dataset used for object recognition, a subset of the 80 million tiny images dataset, consisting of 60,000 32x32 color images containing one of 10 object classes, with 6000 images per class. It was collected by Alex Krizhevsky, Vinod Nair, and Geoffrey Hinton.

Fig. 14.13.1: CIFAR-10 image classification competition webpage information. The data set for the competition can be accessed by clicking the “Data” tab.

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```
import pandas as pd
import shutil
import time
```

### 14.13.1 Obtain and Organize the Data Sets

The competition data is divided into a training set and testing set. The training set contains 50,000 images. The testing set contains 300,000 images, of which 10,000 images are used for scoring, while the other 290,000 non-scoring images are included to prevent the manual labeling of the testing set and the submission of labeling results. The image formats in both data sets are PNG, with heights and widths of 32 pixels and three color channels (RGB). The images cover 10 categories: planes, cars, birds, cats, deer, dogs, frogs, horses, boats, and trucks. The upper-left corner of Figure 11.16 shows some images of planes, cars, and birds in the data set.

#### Download the Data Set

After logging in to Kaggle, we can click on the “Data” tab on the CIFAR-10 image classification competition webpage shown in Figure 11.16 and download the training data set “train.7z”, the testing data set “test.7z”, and the training data set labels “trainlabels.csv”.

#### Unzip the Data Set

The training data set “train.7z” and the test data set “test.7z” need to be unzipped after downloading. After unzipping the data sets, store the training data set, test data set, and training data set labels in the following respective paths:

- ..../data/kaggle\_cifar10/train/[1-50000].png
- ..../data/kaggle\_cifar10/test/[1-300000].png
- ..../data/kaggle\_cifar10/trainLabels.csv

To make it easier to get started, we provide a small-scale sample of the data set mentioned above. “train\_tiny.zip” contains 100 training examples, while “test\_tiny.zip” contains only one test example. Their unzipped folder names are “train\_tiny” and “test\_tiny”, respectively. In addition, unzip the zip file of the training data set labels to obtain the file “trainlabels.csv”. If you are going to use the full data set of the Kaggle competition, you will also need to change the following `demo` variable to `False`.

```
# If you use the full data set downloaded for the Kaggle competition, change
# the demo variable to False
demo = True
if demo:
    import zipfile
    for f in ['train_tiny.zip', 'test_tiny.zip', 'trainLabels.csv.zip']:
        with zipfile.ZipFile('../data/kaggle_cifar10/' + f, 'r') as z:
            z.extractall('../data/kaggle_cifar10/')
```

## Organize the Data Set

We need to organize data sets to facilitate model training and testing. The following `read_label_file` function will be used to read the label file for the training data set. The parameter `valid_ratio` in this function is the ratio of the number of examples in the validation set to the number of examples in the original training set.

```
def read_label_file(data_dir, label_file, train_dir, valid_ratio):
    with open(os.path.join(data_dir, label_file), 'r') as f:
        # Skip the file header line (column name)
        lines = f.readlines()[1:]
        tokens = [l.rstrip().split(',') for l in lines]
        idx_label = dict(((int(idx), label) for idx, label in tokens))
    labels = set(idx_label.values())
    n_train_valid = len(os.listdir(os.path.join(data_dir, train_dir)))
    n_train = int(n_train_valid * (1 - valid_ratio))
    assert 0 < n_train < n_train_valid
    return n_train // len(labels), idx_label
```

Below we define a helper function to create a path only if the path does not already exist.

```
# save to the d2l package.
def mkdir_if_not_exist(path):
    if not os.path.exists(os.path.join(*path)):
        os.makedirs(os.path.join(*path))
```

Next, we define the `reorg_train_valid` function to segment the validation set from the original training set. Here, we use `valid_ratio=0.1` as an example. Since the original training set has 50,000 images, there will be 45,000 images used for training and stored in the path “`input_dir/train`” when tuning hyper-parameters, while the other 5,000 images will be stored as validation set in the path “`input_dir/valid`”. After organizing the data, images of the same type will be placed under the same folder so that we can read them later.

```
def reorg_train_valid(data_dir, train_dir, input_dir, n_train_per_label,
                      idx_label):
    label_count = {}
    for train_file in os.listdir(os.path.join(data_dir, train_dir)):
        idx = int(train_file.split('.')[0])
```

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```

label = idx_label[idx]
mkdir_if_not_exist([data_dir, input_dir, 'train_valid', label])
shutil.copy(os.path.join(data_dir, train_dir, train_file),
            os.path.join(data_dir, input_dir, 'train_valid', label))
if label not in label_count or label_count[label] < n_train_per_label:
    mkdir_if_not_exist([data_dir, input_dir, 'train', label])
    shutil.copy(os.path.join(data_dir, train_dir, train_file),
                os.path.join(data_dir, input_dir, 'train', label))
    label_count[label] = label_count.get(label, 0) + 1
else:
    mkdir_if_not_exist([data_dir, input_dir, 'valid', label])
    shutil.copy(os.path.join(data_dir, train_dir, train_file),
                os.path.join(data_dir, input_dir, 'valid', label))

```

The `reorg_test` function below is used to organize the testing set to facilitate the reading during prediction.

```

def reorg_test(data_dir, test_dir, input_dir):
    mkdir_if_not_exist([data_dir, input_dir, 'test', 'unknown'])
    for test_file in os.listdir(os.path.join(data_dir, test_dir)):
        shutil.copy(os.path.join(data_dir, test_dir, test_file),
                    os.path.join(data_dir, input_dir, 'test', 'unknown'))

```

Finally, we use a function to call the previously defined `reorg_test`, `reorg_train_valid`, and `reorg_test` functions.

```

def reorg_cifar10_data(data_dir, label_file, train_dir, test_dir, input_dir,
                      valid_ratio):
    n_train_per_label, idx_label = read_label_file(data_dir, label_file,
                                                   train_dir, valid_ratio)
    reorg_train_valid(data_dir, train_dir, input_dir, n_train_per_label,
                      idx_label)
    reorg_test(data_dir, test_dir, input_dir)

```

We use only 100 training example and one test example here. The folder names for the training and testing data sets are “train\_tiny” and “test\_tiny”, respectively. Accordingly, we only set the batch size to 1. During actual training and testing, the complete data set of the Kaggle competition should be used and `batch_size` should be set to a larger integer, such as 128. We use 10% of the training examples as the validation set for tuning hyper-parameters.

```

if demo:
    # Note: Here, we use small training sets and small testing sets and the
    # batch size should be set smaller. When using the complete data set for
    # the Kaggle competition, the batch size can be set to a large integer
    train_dir, test_dir, batch_size = 'train_tiny', 'test_tiny', 1
else:
    train_dir, test_dir, batch_size = 'train', 'test', 128
data_dir, label_file = '../data/kaggle_cifar10', 'trainLabels.csv'
input_dir, valid_ratio = 'train_valid_test', 0.1
reorg_cifar10_data(data_dir, label_file, train_dir, test_dir, input_dir,
                  valid_ratio)

```

### 14.13.2 Image Augmentation

To cope with overfitting, we use image augmentation. For example, by adding `transforms.RandomFlipLeftRight()`, the images can be flipped at random. We can also perform normalization for the three RGB channels of color images using `transforms.Normalize()`. Below, we list some of these operations that you can choose to use or modify depending on requirements.

```
transform_train = gluon.data.vision.transforms.Compose([
    # Magnify the image to a square of 40 pixels in both height and width
    gluon.data.vision.transforms.Resize(40),
    # Randomly crop a square image of 40 pixels in both height and width to
    # produce a small square of 0.64 to 1 times the area of the original
    # image, and then shrink it to a square of 32 pixels in both height and
    # width
    gluon.data.vision.transforms.RandomResizedCrop(32, scale=(0.64, 1.0),
                                                   ratio=(1.0, 1.0)),
    gluon.data.vision.transforms.RandomFlipLeftRight(),
    gluon.data.vision.transforms.ToTensor(),
    # Normalize each channel of the image
    gluon.data.vision.transforms.Normalize([0.4914, 0.4822, 0.4465],
                                          [0.2023, 0.1994, 0.2010]))]
```

In order to ensure the certainty of the output during testing, we only perform normalization on the image.

```
transform_test = gluon.data.vision.transforms.Compose([
    gluon.data.vision.transforms.ToTensor(),
    gluon.data.vision.transforms.Normalize([0.4914, 0.4822, 0.4465],
                                          [0.2023, 0.1994, 0.2010]))]
```

### 14.13.3 Read the Data Set

Next, we can create the `ImageFolderDataset` instance to read the organized data set containing the original image files, where each data instance includes the image and label.

```
# Read the original image file. Flag=1 indicates that the input image has
# three channels (color)
train_ds = gluon.data.vision.ImageFolderDataset(
    os.path.join(data_dir, input_dir, 'train'), flag=1)
valid_ds = gluon.data.vision.ImageFolderDataset(
    os.path.join(data_dir, input_dir, 'valid'), flag=1)
train_valid_ds = gluon.data.vision.ImageFolderDataset(
    os.path.join(data_dir, input_dir, 'train_valid'), flag=1)
test_ds = gluon.data.vision.ImageFolderDataset(
    os.path.join(data_dir, input_dir, 'test'), flag=1)
```

We specify the defined image augmentation operation in `DataLoader`. During training, we only use the validation set to evaluate the model, so we need to ensure the certainty of the output. During prediction, we will train the model on the combined training set and validation set to make full use of all labelled data.

```
train_iter = gluon.data.DataLoader(train_ds.transform_first(transform_train),
                                   batch_size, shuffle=True, last_batch='keep')
valid_iter = gluon.data.DataLoader(valid_ds.transform_first(transform_test),
```

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```

        batch_size, shuffle=True, last_batch='keep')
train_valid_iter = gluon.data.DataLoader(train_valid_ds.transform_first(
    transform_train), batch_size, shuffle=True, last_batch='keep')
test_iter = gluon.data.DataLoader(test_ds.transform_first(transform_test),
                                 batch_size, shuffle=False, last_batch='keep')

```

#### 14.13.4 Define the Model

Here, we build the residual blocks based on the HybridBlock class, which is slightly different than the implementation described in Section 9.6. This is done to improve execution efficiency.

```

class Residual(nn.HybridBlock):
    def __init__(self, num_channels, use_1x1conv=False, strides=1, **kwargs):
        super(Residual, self).__init__(**kwargs)
        self.conv1 = nn.Conv2D(num_channels, kernel_size=3, padding=1,
                            strides=strides)
        self.conv2 = nn.Conv2D(num_channels, kernel_size=3, padding=1)
        if use_1x1conv:
            self.conv3 = nn.Conv2D(num_channels, kernel_size=1,
                                strides=strides)
        else:
            self.conv3 = None
        self.bn1 = nn.BatchNorm()
        self.bn2 = nn.BatchNorm()

    def hybrid_forward(self, F, X):
        Y = F.relu(self.bn1(self.conv1(X)))
        Y = self.bn2(self.conv2(Y))
        if self.conv3:
            X = self.conv3(X)
        return F.relu(Y + X)

```

Next, we define the ResNet-18 model.

```

def resnet18(num_classes):
    net = nn.HybridSequential()
    net.add(nn.Conv2D(64, kernel_size=3, strides=1, padding=1),
           nn.BatchNorm(), nn.Activation('relu'))

    def resnet_block(num_channels, num_residuals, first_block=False):
        blk = nn.HybridSequential()
        for i in range(num_residuals):
            if i == 0 and not first_block:
                blk.add(Residual(num_channels, use_1x1conv=True, strides=2))
            else:
                blk.add(Residual(num_channels))
        return blk

    net.add(resnet_block(64, 2, first_block=True),
            resnet_block(128, 2),
            resnet_block(256, 2),

```

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```

    resnet_block(512, 2))
net.add(nn.GlobalAvgPool2D(), nn.Dense(num_classes))
return net

```

The CIFAR-10 image classification challenge uses 10 categories. We will perform Xavier random initialization on the model before training begins.

```

def get_net(ctx):
    num_classes = 10
    net = resnet18(num_classes)
    net.initialize(ctx=ctx, init=init.Xavier())
    return net

loss = gluon.loss.SoftmaxCrossEntropyLoss()

```

### 14.13.5 Define the Training Functions

We will select the model and tune hyper-parameters according to the model's performance on the validation set. Next, we define the model training function `train`. We record the training time of each epoch, which helps us compare the time costs of different models.

```

def train(net, train_iter, valid_iter, num_epochs, lr, wd, ctx, lr_period,
         lr_decay):
    trainer = gluon.Trainer(net.collect_params(), 'sgd',
                            {'learning_rate': lr, 'momentum': 0.9, 'wd': wd})
    for epoch in range(num_epochs):
        train_l_sum, train_acc_sum, n, start = 0.0, 0.0, 0, time.time()
        if epoch > 0 and epoch % lr_period == 0:
            trainer.set_learning_rate(trainer.learning_rate * lr_decay)
        for X, y in train_iter:
            y = y.astype('float32').as_in_context(ctx)
            with autograd.record():
                y_hat = net(X.as_in_context(ctx))
                l = loss(y_hat, y).sum()
            l.backward()
            trainer.step(batch_size)
            train_l_sum += l.asscalar()
            train_acc_sum += (y_hat.argmax(axis=1) == y).sum().asscalar()
            n += y.size
        time_s = "time %.2f sec" % (time.time() - start)
        if valid_iter is not None:
            valid_acc = d2l.evaluate_accuracy_gpu(net, valid_iter)
            epoch_s = ("epoch %d, loss %f, train acc %f, valid acc %f, "
                      "% (epoch + 1, train_l_sum / n, train_acc_sum / n,
                      valid_acc)")
        else:
            epoch_s = ("epoch %d, loss %f, train acc %f, " %
                      (epoch + 1, train_l_sum / n, train_acc_sum / n))
        print(epoch_s + time_s + ', lr ' + str(trainer.learning_rate))

```

### 14.13.6 Train and Validate the Model

Now, we can train and validate the model. The following hyper-parameters can be tuned. For example, we can increase the number of epochs. Because `lr_period` and `lr_decay` are set to 80 and 0.1 respectively, the learning rate of the optimization algorithm will be multiplied by 0.1 after every 80 epochs. For simplicity, we only train one epoch here.

```
ctx, num_epochs, lr, wd = d2l.try_gpu(), 1, 0.1, 5e-4
lr_period, lr_decay, net = 80, 0.1, get_net(ctx)
net.hybridize()
train(net, train_iter, valid_iter, num_epochs, lr, wd, ctx, lr_period,
      lr_decay)
```

```
epoch 1, loss 6.009422, train acc 0.088889, valid acc 0.000000, time 1.30 sec, lr 0.1
```

### 14.13.7 Classify the Testing Set and Submit Results on Kaggle

After obtaining a satisfactory model design and hyper-parameters, we use all training data sets (including validation sets) to retrain the model and classify the testing set.

```
net, preds = get_net(ctx), []
net.hybridize()
train(net, train_valid_iter, None, num_epochs, lr, wd, ctx, lr_period,
      lr_decay)

for X, _ in test_iter:
    y_hat = net(X.as_in_context(ctx))
    preds.extend(y_hat.argmax(axis=1).astype(int).asnumpy())
sorted_ids = list(range(1, len(test_ds) + 1))
sorted_ids.sort(key=lambda x: str(x))
df = pd.DataFrame({'id': sorted_ids, 'label': preds})
df['label'] = df['label'].apply(lambda x: train_valid_ds.synsets[x])
df.to_csv('submission.csv', index=False)
```

```
epoch 1, loss 5.894879, train acc 0.070000, time 1.20 sec, lr 0.1
```

After executing the above code, we will get a “`submission.csv`” file. The format of this file is consistent with the Kaggle competition requirements. The method for submitting results is similar to method in Section 6.10.

### 14.13.8 Summary

- We can create an `ImageFolderDataset` instance to read the data set containing the original image files.
- We can use convolutional neural networks, image augmentation, and hybrid programming to take part in an image classification competition.

### 14.13.9 Exercises

- Use the complete CIFAR-10 data set for the Kaggle competition. Change the `batch_size` and number of epochs `num_epochs` to 128 and 100, respectively. See what accuracy and ranking you can achieve in this competition.
- What accuracy can you achieve when not using image augmentation?
- Scan the QR code to access the relevant discussions and exchange ideas about the methods used and the results obtained with the community. Can you come up with any better techniques?

### 14.13.10 Scan the QR Code to Discuss<sup>192</sup>



## 14.14 Dog Breed Identification (ImageNet Dogs) on Kaggle

In this section, we will tackle the dog breed identification challenge in the Kaggle Competition. The competition's web address is

<https://www.kaggle.com/c/dog-breed-identification>

In this competition, we attempt to identify 120 different breeds of dogs. The data set used in this competition is actually a subset of the famous ImageNet data set. Different from the images in the CIFAR-10 data set used in the previous section, the images in the ImageNet data set are higher and wider and their dimensions are inconsistent.

Fig. 14.14.1 shows the information on the competition's webpage. In order to submit the results, please register an account on the Kaggle website first.

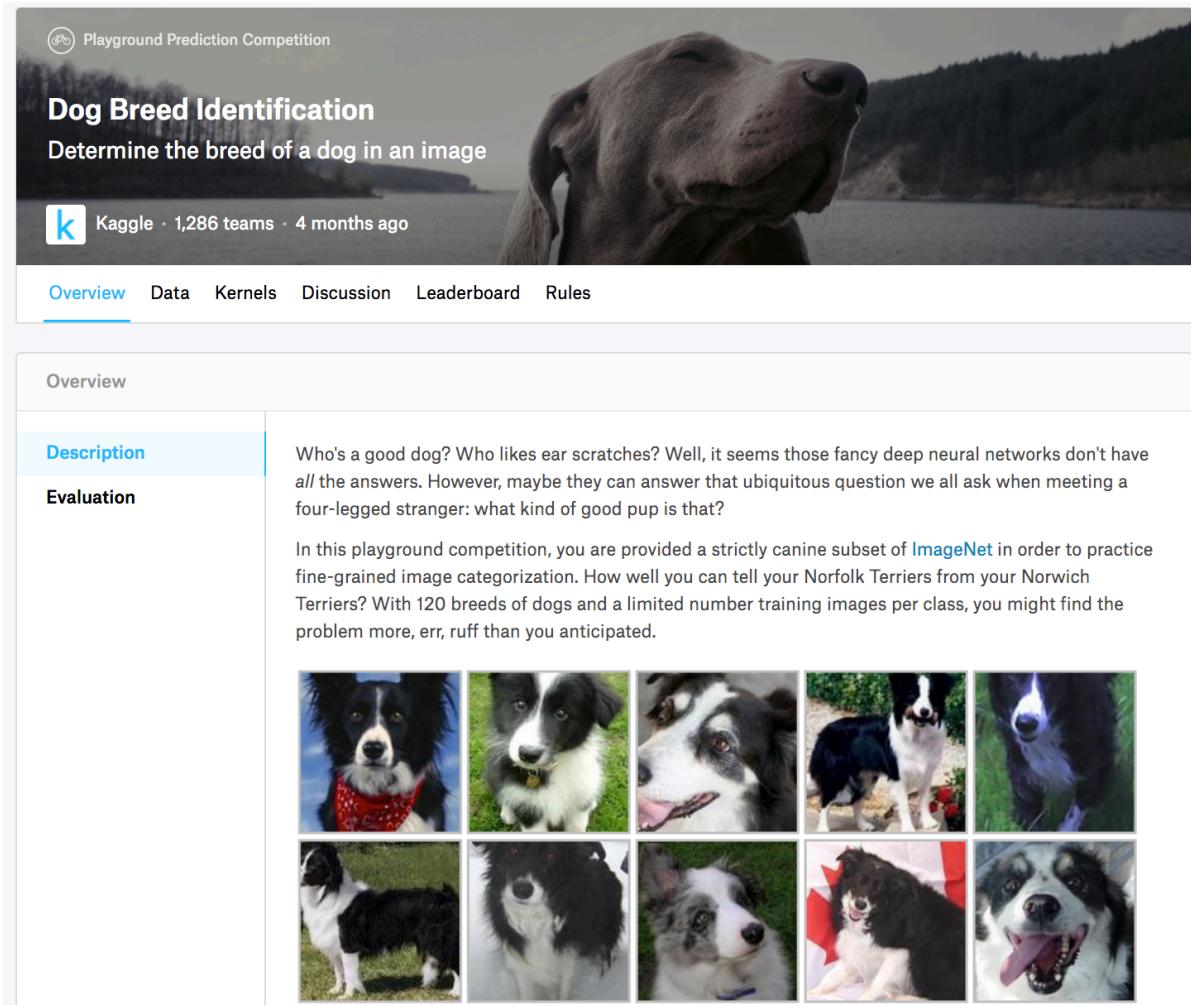
First, import the packages or modules required for the competition.

```
import collections
import d2l
import math
from mxnet import autograd, gluon, init, nd
from mxnet.gluon import nn
import os
import shutil
import time
import zipfile
```

### 14.14.1 Obtain and Organize the Data Sets

The competition data is divided into a training set and testing set. The training set contains 10,222 images and the testing set contains 10,357 images. The images in both sets are in JPEG format. These images

<sup>192</sup> <https://discuss.mxnet.io/t/2450>



The screenshot shows the Kaggle Dog Breed Identification competition page. At the top, there's a header with the competition name, a thumbnail of a dog, and a 'Kaggle' badge indicating 1,286 teams participated 4 months ago. Below the header are navigation links for Overview, Data, Kernels, Discussion, Leaderboard, and Rules. The 'Overview' tab is currently selected. The main content area has two sections: 'Description' and 'Evaluation'. The 'Description' section contains a paragraph about the competition's purpose and the 'Evaluation' section contains a paragraph about the data set and its use for fine-grained categorization. Below these sections is a grid of 10 small images showing various dogs, which serves as a preview of the data set.

Fig. 14.14.1: Dog breed identification competition website. The data set for the competition can be accessed by clicking the “Data” tab.

contain three RGB channels (color) and they have different heights and widths. There are 120 breeds of dogs in the training set, including Labradors, Poodles, Dachshunds, Samoyeds, Huskies, Chihuahuas, and Yorkshire Terriers.

## Download the Data Set

After logging in to Kaggle, we can click on the “Data” tab on the dog breed identification competition webpage shown in Fig. 14.14.1 and download the training data set “train.zip”, the testing data set “test.zip”, and the training data set labels “label.csv.zip”. After downloading the files, place them in the three paths below:

- ..../data/kaggle\_dog/train.zip
- ..../data/kaggle\_dog/test.zip
- ..../data/kaggle\_dog/labels.csv.zip

To make it easier to get started, we provide a small-scale sample of the data set mentioned above, “train\_valid\_test\_tiny.zip”. If you are going to use the full data set for the Kaggle competition, you will also need to change the `demo` variable below to `False`.

```
# If you use the full data set downloaded for the Kaggle competition, change
# the variable below to False
demo = True
data_dir = '../data/kaggle_dog'
if demo:
    zipfiles = ['train_valid_test_tiny.zip']
else:
    zipfiles = ['train.zip', 'test.zip', 'labels.csv.zip']
for f in zipfiles:
    with zipfile.ZipFile(data_dir + '/' + f, 'r') as z:
        z.extractall(data_dir)
```

## Organize the Data Set

Next, we define the `reorg_train_valid` function to segment the validation set from the original Kaggle competition training set. The parameter `valid_ratio` in this function is the ratio of the number of examples of each dog breed in the validation set to the number of examples of the breed with the least examples (66) in the original training set. After organizing the data, images of the same breed will be placed in the same folder so that we can read them later.

```
def reorg_train_valid(data_dir, train_dir, input_dir, valid_ratio, idx_label):
    # The number of examples of the least represented breed in the training
    # set
    min_n_train_per_label = (
        collections.Counter(idx_label.values()).most_common()[:-2:-1][0][1])
    # The number of examples of each breed in the validation set
    n_valid_per_label = math.floor(min_n_train_per_label * valid_ratio)
    label_count = {}
    for train_file in os.listdir(os.path.join(data_dir, train_dir)):
        idx = train_file.split('.')[0]
        label = idx_label[idx]
        d2l.mkdir_if_not_exist([data_dir, input_dir, 'train_valid', label])
        shutil.copy(os.path.join(data_dir, train_dir, train_file),
                    os.path.join(data_dir, input_dir, 'train_valid', label))
```

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```

if label not in label_count or label_count[label] < n_valid_per_label:
    d2l.mkdir_if_not_exist([data_dir, input_dir, 'valid', label])
    shutil.copy(os.path.join(data_dir, train_dir, train_file),
                os.path.join(data_dir, input_dir, 'valid', label))
    label_count[label] = label_count.get(label, 0) + 1
else:
    d2l.mkdir_if_not_exist([data_dir, input_dir, 'train', label])
    shutil.copy(os.path.join(data_dir, train_dir, train_file),
                os.path.join(data_dir, input_dir, 'train', label))

```

The `reorg_dog_data` function below is used to read the training data labels, segment the validation set, and organize the training set.

```

def reorg_dog_data(data_dir, label_file, train_dir, test_dir, input_dir,
                   valid_ratio):
    # Read the training data labels
    with open(os.path.join(data_dir, label_file), 'r') as f:
        # Skip the file header line (column name)
        lines = f.readlines()[1:]
        tokens = [l.rstrip().split(',') for l in lines]
        idx_label = dict(((idx, label) for idx, label in tokens))
    reorg_train_valid(data_dir, train_dir, input_dir, valid_ratio, idx_label)
    # Organize the training set
    d2l.mkdir_if_not_exist([data_dir, input_dir, 'test', 'unknown'])
    for test_file in os.listdir(os.path.join(data_dir, test_dir)):
        shutil.copy(os.path.join(data_dir, test_dir, test_file),
                    os.path.join(data_dir, input_dir, 'test', 'unknown'))

```

Because we are using a small data set, we set the batch size to 1. During actual training and testing, we would use the entire Kaggle Competition data set and call the `reorg_dog_data` function to organize the data set. Likewise, we would need to set the `batch_size` to a larger integer, such as 128.

```

if demo:
    # Note: Here, we use a small data set and the batch size should be set
    # smaller. When using the complete data set for the Kaggle competition, we
    # can set the batch size to a larger integer
    input_dir, batch_size = 'train_valid_test_tiny', 1
else:
    label_file, train_dir, test_dir = 'labels.csv', 'train', 'test'
    input_dir, batch_size, valid_ratio = 'train_valid_test', 128, 0.1
    reorg_dog_data(data_dir, label_file, train_dir, test_dir, input_dir,
                   valid_ratio)

```

## 14.14.2 Image Augmentation

The size of the images in this section are larger than the images in the previous section. Here are some more image augmentation operations that might be useful.

```

transform_train = gluon.data.vision.transforms.Compose([
    # Randomly crop the image to obtain an image with an area of 0.08 to 1 of
    # the original area and height to width ratio between 3/4 and 4/3. Then,

```

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```
# scale the image to create a new image with a height and width of 224
# pixels each
gluon.data.vision.transforms.RandomResizedCrop(224, scale=(0.08, 1.0),
                                                ratio=(3.0/4.0, 4.0/3.0)),
gluon.data.vision.transforms.RandomFlipLeftRight(),
# Randomly change the brightness, contrast, and saturation
gluon.data.vision.transforms.RandomColorJitter(brightness=0.4, contrast=0.4,
                                                saturation=0.4),
# Add random noise
gluon.data.vision.transforms.RandomLighting(0.1),
gluon.data.vision.transforms.ToTensor(),
# Standardize each channel of the image
gluon.data.vision.transforms.Normalize([0.485, 0.456, 0.406],
                                       [0.229, 0.224, 0.225]))
```

During testing, we only use definite image preprocessing operations.

```
transform_test = gluon.data.vision.transforms.Compose([
    gluon.data.vision.transforms.Resize(256),
    # Crop a square of 224 by 224 from the center of the image
    gluon.data.vision.transforms.CenterCrop(224),
    gluon.data.vision.transforms.ToTensor(),
    gluon.data.vision.transforms.Normalize([0.485, 0.456, 0.406],
                                           [0.229, 0.224, 0.225]))
```

### 14.14.3 Read the Data Set

As in the previous section, we can create an `ImageFolderDataset` instance to read the data set containing the original image files.

```
train_ds = gluon.data.vision.ImageFolderDataset(
    os.path.join(data_dir, input_dir, 'train'), flag=1)
valid_ds = gluon.data.vision.ImageFolderDataset(
    os.path.join(data_dir, input_dir, 'valid'), flag=1)
train_valid_ds = gluon.data.vision.ImageFolderDataset(
    os.path.join(data_dir, input_dir, 'train_valid'), flag=1)
test_ds = gluon.data.vision.ImageFolderDataset(
    os.path.join(data_dir, input_dir, 'test'), flag=1)
```

Here, we create a `DataLoader` instance, just like in the previous section.

```
train_iter = gluon.data.DataLoader(train_ds.transform_first(transform_train),
                                    batch_size, shuffle=True, last_batch='keep')
valid_iter = gluon.data.DataLoader(valid_ds.transform_first(transform_test),
                                    batch_size, shuffle=True, last_batch='keep')
train_valid_iter = gluon.data.DataLoader(train_valid_ds.transform_first(
    transform_train), batch_size, shuffle=True, last_batch='keep')
test_iter = gluon.data.DataLoader(test_ds.transform_first(transform_test),
                                 batch_size, shuffle=False, last_batch='keep')
```

#### 14.14.4 Define the Model

The data set for this competition is a subset of the ImageNet data set. Therefore, we can use the approach discussed in Section 14.2 to select a model pre-trained on the entire ImageNet data set and use it to extract image features to be input in the custom small-scale output network. Gluon provides a wide range of pre-trained models. Here, we will use the pre-trained ResNet-34 model. Because the competition data set is a subset of the pre-training data set, we simply reuse the input of the pre-trained model's output layer, i.e. the extracted features. Then, we can replace the original output layer with a small custom output network that can be trained, such as two fully connected layers in a series. Different from the experiment in Section 14.2, here, we do not retrain the pre-trained model used for feature extraction. This reduces the training time and the memory required to store model parameter gradients.

You must note that, during image augmentation, we use the mean values and standard deviations of the three RGB channels for the entire ImageNet data set for normalization. This is consistent with the normalization of the pre-trained model.

```
def get_net(ctx):
    finetune_net = gluon.model_zoo.vision.resnet34_v2(pretrained=True)
    # Define a new output network
    finetune_net.output_new = nn.HybridSequential(prefix='')
    finetune_net.output_new.add(nn.Dense(256, activation='relu'))
    # There are 120 output categories
    finetune_net.output_new.add(nn.Dense(120))
    # Initialize the output network
    finetune_net.output_new.initialize(init.Xavier(), ctx=ctx)
    # Distribute the model parameters to the CPUs or GPUs used for computation
    finetune_net.collect_params().reset_ctx(ctx)
    return finetune_net
```

When calculating the loss, we first use the member variable `features` to obtain the input of the pre-trained model's output layer, i.e. the extracted feature. Then, we use this feature as the input for our small custom output network and compute the output.

```
loss = gluon.loss.SoftmaxCrossEntropyLoss()

def evaluate_loss(data_iter, net, ctx):
    l_sum, n = 0.0, 0
    for X, y in data_iter:
        y = y.as_in_context(ctx)
        output_features = net.features(X.as_in_context(ctx))
        outputs = net.output_new(output_features)
        l_sum += loss(outputs, y).sum().asscalar()
        n += y.size
    return l_sum / n
```

#### 14.14.5 Define the Training Functions

We will select the model and tune hyper-parameters according to the model's performance on the validation set. The model training function `train` only trains the small custom output network.

```
def train(net, train_iter, valid_iter, num_epochs, lr, wd, ctx, lr_period,
          lr_decay):
    # Only train the small custom output network
```

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```

trainer = gluon.Trainer(net.output_new.collect_params(), 'sgd',
                        {'learning_rate': lr, 'momentum': 0.9, 'wd': wd})
for epoch in range(num_epochs):
    train_l_sum, n, start = 0.0, 0, time.time()
    if epoch > 0 and epoch % lr_period == 0:
        trainer.set_learning_rate(trainer.learning_rate * lr_decay)
    for X, y in train_iter:
        y = y.as_in_context(ctx)
        output_features = net.features(X.as_in_context(ctx))
        with autograd.record():
            outputs = net.output_new(output_features)
            l = loss(outputs, y).sum()
        l.backward()
        trainer.step(batch_size)
        train_l_sum += l.asscalar()
        n += y.size
    time_s = "time %.2f sec" % (time.time() - start)
    if valid_iter is not None:
        valid_loss = evaluate_loss(valid_iter, net, ctx)
        epoch_s = ("epoch %d, train loss %f, valid loss %f, "
                   % (epoch + 1, train_l_sum / n, valid_loss))
    else:
        epoch_s = ("epoch %d, train loss %f, "
                   % (epoch + 1, train_l_sum / n))
    print(epoch_s + time_s + ', lr ' + str(trainer.learning_rate))

```

#### 14.14.6 Train and Validate the Model

Now, we can train and validate the model. The following hyper-parameters can be tuned. For example, we can increase the number of epochs. Because `lr_period` and `lr_decay` are set to 10 and 0.1 respectively, the learning rate of the optimization algorithm will be multiplied by 0.1 after every 10 epochs.

```

ctx, num_epochs, lr, wd = d2l.try_gpu(), 1, 0.01, 1e-4
lr_period, lr_decay, net = 10, 0.1, get_net(ctx)
net.hybridize()
train(net, train_iter, valid_iter, num_epochs, lr, wd, ctx, lr_period,
      lr_decay)

```

```
epoch 1, train loss 5.228812, valid loss 4.799443, time 1.58 sec, lr 0.01
```

#### 14.14.7 Classify the Testing Set and Submit Results on Kaggle

After obtaining a satisfactory model design and hyper-parameters, we use all training data sets (including validation sets) to retrain the model and then classify the testing set. Note that predictions are made by the output network we just trained.

```

net = get_net(ctx)
net.hybridize()
train(net, train_valid_iter, None, num_epochs, lr, wd, ctx, lr_period,
      lr_decay)

```

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```

lr_decay)

preds = []
for data, label in test_iter:
    output_features = net.features(data.as_in_context(ctx))
    output = nd.softmax(net.output_new(output_features))
    preds.extend(output.astype(np.float32))
ids = sorted(os.listdir(os.path.join(data_dir, input_dir, 'test/unknown')))
with open('submission.csv', 'w') as f:
    f.write('id,' + ','.join(train_valid_ds.synsets) + '\n')
    for i, output in zip(ids, preds):
        f.write(i.split('.')[0] + ',' + ','.join(
            [str(num) for num in output]) + '\n')

```

```
epoch 1, train loss 5.084524, time 2.70 sec, lr 0.01
```

After executing the above code, we will generate a “`submission.csv`” file. The format of this file is consistent with the Kaggle competition requirements. The method for submitting results is similar to method in Section 6.10.

#### 14.14.8 Summary

- We can use a model pre-trained on the ImageNet data set to extract features and only train a small custom output network. This will allow us to classify a subset of the ImageNet data set with lower computing and storage overhead.

#### 14.14.9 Exercises

- When using the entire Kaggle data set, what kind of results do you get when you increase the `batch_size` (batch size) and `num_epochs` (number of epochs)?
- Do you get better results if you use a deeper pre-trained model?
- Scan the QR code to access the relevant discussions and exchange ideas about the methods used and the results obtained with the community. Can you come up with any better techniques?

#### 14.14.10 Scan the QR Code to Discuss<sup>193</sup>



<sup>193</sup> <https://discuss.mxnet.io/t/2451>

## NATURAL LANGUAGE PROCESSING

Natural language processing is concerned with interactions between computers and humans that use natural language. In practice, it is very common for us to use this technique to process and analyze large amounts of natural language data, like the language models from the “Recurrent Neural Networks” section.

In this chapter, we will discuss how to use vectors to represent words and train the word vectors on a corpus. We will also use word vectors pre-trained on a larger corpus to find synonyms and analogies. Then, in the text classification task, we will use word vectors to analyze the emotion of a text and explain the important ideas of timing data classification based on RNNs and the convolutional neural networks. In addition, many of the outputs of natural language processing tasks are not fixed, such as sentences of arbitrary length. We will introduce the encoder-decoder model, beam search, and attention mechanisms to address problems of this type and apply them to machine translation.

### 15.1 Word Embedding (word2vec)

A natural language is a complex system that we use to communicate. Words are commonly used as the unit of analysis in natural language processing. As its name implies, a word vector is a vector used to represent a word. It can also be thought of as the feature vector of a word. The technique of mapping words to vectors of real numbers is also known as word embedding. Over the last few years, word embedding has gradually become basic knowledge in natural language processing.

#### 15.1.1 Why not Use One-hot Vectors?

We used one-hot vectors to represent words (characters are words) in Section 10.5 . Recall that when we assume the number of different words in a dictionary (the dictionary size) is  $N$ , each word can correspond one-to-one with consecutive integers from 0 to  $N - 1$ . These integers that correspond to words are called the indices of the words. We assume that the index of a word is  $i$ . In order to get the one-hot vector representation of the word, we create a vector of all 0s with a length of  $N$  and set element  $i$  to 1. In this way, each word is represented as a vector of length  $N$  that can be used directly by the neural network.

Although one-hot word vectors are easy to construct, they are usually not a good choice. One of the major reasons is that the one-hot word vectors cannot accurately express the similarity between different words, such as the cosine similarity that we commonly use. For the vectors  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ , their cosine similarities are the cosines of the angles between them:

$$\frac{\mathbf{x}^\top \mathbf{y}}{\|\mathbf{x}\| \|\mathbf{y}\|} \in [-1, 1]. \quad (15.1.1)$$

Since the cosine similarity between the one-hot vectors of any two different words is 0, it is difficult to use the one-hot vector to accurately represent the similarity between multiple different words.

Word2vec<sup>194</sup> is a tool that we came up with to solve the problem above. It represents each word with a fixed-length vector and uses these vectors to better indicate the similarity and analogy relationships between different words. The Word2vec tool contains two models: skip-gram [47] and continuous bag of words (CBOW) [46]. Next, we will take a look at the two models and their training methods.

### 15.1.2 The Skip-Gram Model

The skip-gram model assumes that a word can be used to generate the words that surround it in a text sequence. For example, we assume that the text sequence is “the”, “man”, “loves”, “his”, and “son”. We use “loves” as the central target word and set the context window size to 2. As shown in Figure 12.1, given the central target word “loves”, the skip-gram model is concerned with the conditional probability for generating the context words, “the”, “man”, “his” and “son”, that are within a distance of no more than 2 words, which is

$$\mathbb{P}(\text{"the"}, \text{"man"}, \text{"his"}, \text{"son"} \mid \text{"loves"}). \quad (15.1.2)$$

We assume that, given the central target word, the context words are generated independently of each other. In this case, the formula above can be rewritten as

$$\mathbb{P}(\text{"the"} \mid \text{"loves"}) \cdot \mathbb{P}(\text{"man"} \mid \text{"loves"}) \cdot \mathbb{P}(\text{"his"} \mid \text{"loves"}) \cdot \mathbb{P}(\text{"son"} \mid \text{"loves"}). \quad (15.1.3)$$

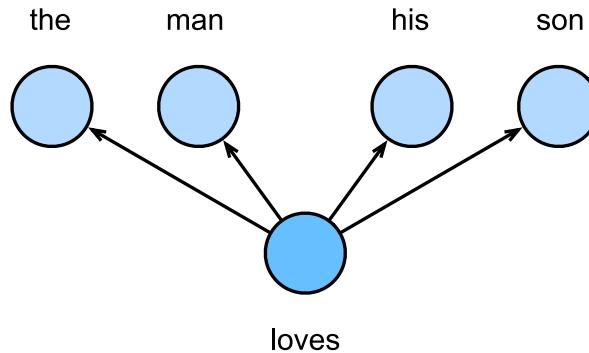


Fig. 15.1.1: The skip-gram model cares about the conditional probability of generating context words for a given central target word.

In the skip-gram model, each word is represented as two  $d$ -dimension vectors, which are used to compute the conditional probability. We assume that the word is indexed as  $i$  in the dictionary, its vector is represented as  $\mathbf{v}_i \in \mathbb{R}^d$  when it is the central target word, and  $\mathbf{u}_i \in \mathbb{R}^d$  when it is a context word. Let the central target word  $w_c$  and context word  $w_o$  be indexed as  $c$  and  $o$  respectively in the dictionary. The conditional probability of generating the context word for the given central target word can be obtained by performing a softmax operation on the vector inner product:

$$\mathbb{P}(w_o \mid w_c) = \frac{\exp(\mathbf{u}_o^\top \mathbf{v}_c)}{\sum_{i \in \mathcal{V}} \exp(\mathbf{u}_i^\top \mathbf{v}_c)}, \quad (15.1.4)$$

where vocabulary index set  $\mathcal{V} = \{0, 1, \dots, |\mathcal{V}| - 1\}$ . Assume that a text sequence of length  $T$  is given, where the word at time step  $t$  is denoted as  $w^{(t)}$ . Assume that context words are independently generated given

<sup>194</sup> <https://code.google.com/archive/p/word2vec/>

center words. When context window size is  $m$ , the likelihood function of the skip-gram model is the joint probability of generating all the context words given any center word

$$\prod_{t=1}^T \prod_{-m \leq j \leq m, j \neq 0} \mathbb{P}(w^{(t+j)} | w^{(t)}), \quad (15.1.5)$$

Here, any time step that is less than 1 or greater than  $T$  can be ignored.

### Skip-Gram Model Training

The skip-gram model parameters are the central target word vector and context word vector for each individual word. In the training process, we are going to learn the model parameters by maximizing the likelihood function, which is also known as maximum likelihood estimation. This is equivalent to minimizing the following loss function:

$$-\sum_{t=1}^T \sum_{-m \leq j \leq m, j \neq 0} \log \mathbb{P}(w^{(t+j)} | w^{(t)}). \quad (15.1.6)$$

If we use the SGD, in each iteration we are going to pick a shorter subsequence through random sampling to compute the loss for that subsequence, and then compute the gradient to update the model parameters. The key of gradient computation is to compute the gradient of the logarithmic conditional probability for the central word vector and the context word vector. By definition, we first have

$$\log \mathbb{P}(w_o | w_c) = \mathbf{u}_o^\top \mathbf{v}_c - \log \left( \sum_{i \in \mathcal{V}} \exp(\mathbf{u}_i^\top \mathbf{v}_c) \right) \quad (15.1.7)$$

Through differentiation, we can get the gradient  $\mathbf{v}_c$  from the formula above.

$$\begin{aligned} \frac{\partial \log \mathbb{P}(w_o | w_c)}{\partial \mathbf{v}_c} &= \mathbf{u}_o - \frac{\sum_{j \in \mathcal{V}} \exp(\mathbf{u}_j^\top \mathbf{v}_c) \mathbf{u}_j}{\sum_{i \in \mathcal{V}} \exp(\mathbf{u}_i^\top \mathbf{v}_c)} \\ &= \mathbf{u}_o - \sum_{j \in \mathcal{V}} \left( \frac{\exp(\mathbf{u}_j^\top \mathbf{v}_c)}{\sum_{i \in \mathcal{V}} \exp(\mathbf{u}_i^\top \mathbf{v}_c)} \right) \mathbf{u}_j \\ &= \mathbf{u}_o - \sum_{j \in \mathcal{V}} \mathbb{P}(w_j | w_c) \mathbf{u}_j. \end{aligned} \quad (15.1.8)$$

Its computation obtains the conditional probability for all the words in the dictionary given the central target word  $w_c$ . We then use the same method to obtain the gradients for other word vectors.

After the training, for any word in the dictionary with index  $i$ , we are going to get its two word vector sets  $\mathbf{v}_i$  and  $\mathbf{u}_i$ . In applications of natural language processing (NLP), the central target word vector in the skip-gram model is generally used as the representation vector of a word.

### 15.1.3 The Continuous Bag Of Words (CBOW) Model

The continuous bag of words (CBOW) model is similar to the skip-gram model. The biggest difference is that the CBOW model assumes that the central target word is generated based on the context words before and after it in the text sequence. With the same text sequence “the”, “man”, “loves”, “his” and “son”, in which “loves” is the central target word, given a context window size of 2, the CBOW model is concerned with the conditional probability of generating the target word “loves” based on the context words “the”, “man”, “his” and “son”(as shown in Figure 12.2), such as

$$\mathbb{P}(\text{"loves"} | \text{"the"}, \text{"man"}, \text{"his"}, \text{"son"}). \quad (15.1.9)$$

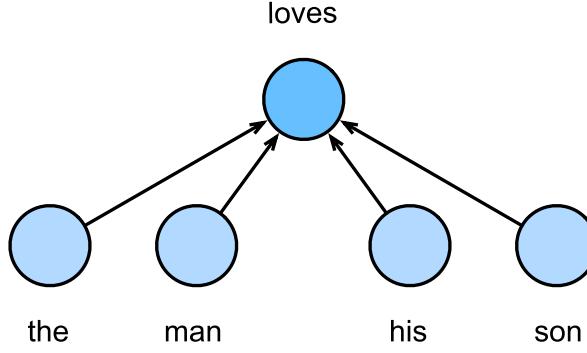


Fig. 15.1.2: The CBOW model cares about the conditional probability of generating the central target word from given context words.

Since there are multiple context words in the CBOW model, we will average their word vectors and then use the same method as the skip-gram model to compute the conditional probability. We assume that  $\mathbf{v}_i \in \mathbb{R}^d$  and  $\mathbf{u}_i \in \mathbb{R}^d$  are the context word vector and central target word vector of the word with index  $i$  in the dictionary (notice that the symbols are opposite to the ones in the skip-gram model). Let central target word  $w_c$  be indexed as  $c$ , and context words  $w_{o_1}, \dots, w_{o_{2m}}$  be indexed as  $o_1, \dots, o_{2m}$  in the dictionary. Thus, the conditional probability of generating a central target word from the given context word is

$$\mathbb{P}(w_c | w_{o_1}, \dots, w_{o_{2m}}) = \frac{\exp\left(\frac{1}{2m}\mathbf{u}_c^\top(\mathbf{v}_{o_1} + \dots + \mathbf{v}_{o_{2m}})\right)}{\sum_{i \in \mathcal{V}} \exp\left(\frac{1}{2m}\mathbf{u}_i^\top(\mathbf{v}_{o_1} + \dots + \mathbf{v}_{o_{2m}})\right)}. \quad (15.1.10)$$

For brevity, denote  $\mathcal{W}_o = \{w_{o_1}, \dots, w_{o_{2m}}\}$ , and  $\bar{\mathbf{v}}_o = (\mathbf{v}_{o_1} + \dots + \mathbf{v}_{o_{2m}})/(2m)$ . The equation above can be simplified as

$$\mathbb{P}(w_c | \mathcal{W}_o) = \frac{\exp(\mathbf{u}_c^\top \bar{\mathbf{v}}_o)}{\sum_{i \in \mathcal{V}} \exp(\mathbf{u}_i^\top \bar{\mathbf{v}}_o)}. \quad (15.1.11)$$

Given a text sequence of length  $T$ , we assume that the word at time step  $t$  is  $w^{(t)}$ , and the context window size is  $m$ . The likelihood function of the CBOW model is the probability of generating any central target word from the context words.

$$\prod_{t=1}^T \mathbb{P}(w^{(t)} | w^{(t-m)}, \dots, w^{(t-1)}, w^{(t+1)}, \dots, w^{(t+m)}). \quad (15.1.12)$$

### CBOB Model Training

CBOB model training is quite similar to skip-gram model training. The maximum likelihood estimation of the CBOB model is equivalent to minimizing the loss function.

$$-\sum_{t=1}^T \log \mathbb{P}(w^{(t)} | w^{(t-m)}, \dots, w^{(t-1)}, w^{(t+1)}, \dots, w^{(t+m)}). \quad (15.1.13)$$

Notice that

$$\log \mathbb{P}(w_c | \mathcal{W}_o) = \mathbf{u}_c^\top \bar{\mathbf{v}}_o - \log \left( \sum_{i \in \mathcal{V}} \exp(\mathbf{u}_i^\top \bar{\mathbf{v}}_o) \right). \quad (15.1.14)$$

Through differentiation, we can compute the logarithm of the conditional probability of the gradient of any context word vector  $\mathbf{v}_{o_i}$  ( $i = 1, \dots, 2m$ ) in the formula above.

$$\frac{\partial \log \mathbb{P}(w_c | \mathcal{W}_o)}{\partial \mathbf{v}_{o_i}} = \frac{1}{2m} \left( \mathbf{u}_c - \sum_{j \in \mathcal{V}} \frac{\exp(\mathbf{u}_j^\top \bar{\mathbf{v}}_o) \mathbf{u}_j}{\sum_{i \in \mathcal{V}} \exp(\mathbf{u}_i^\top \bar{\mathbf{v}}_o)} \right) = \frac{1}{2m} \left( \mathbf{u}_c - \sum_{j \in \mathcal{V}} \mathbb{P}(w_j | \mathcal{W}_o) \mathbf{u}_j \right). \quad (15.1.15)$$

We then use the same method to obtain the gradients for other word vectors. Unlike the skip-gram model, we usually use the context word vector as the representation vector for a word in the CBOW model.

### 15.1.4 Summary

- A word vector is a vector used to represent a word. The technique of mapping words to vectors of real numbers is also known as word embedding.
- Word2vec includes both the continuous bag of words (CBOW) and skip-gram models. The skip-gram model assumes that context words are generated based on the central target word. The CBOW model assumes that the central target word is generated based on the context words.

### 15.1.5 Exercises

- What is the computational complexity of each gradient? If the dictionary contains a large volume of words, what problems will this cause?
- There are some fixed phrases in the English language which consist of multiple words, such as “new york”. How can you train their word vectors? Hint: See section 4 in the Word2vec paper[2].
- Use the skip-gram model as an example to think about the design of a word2vec model. What is the relationship between the inner product of two word vectors and the cosine similarity in the skip-gram model? For a pair of words with close semantical meaning, why it is likely for their word vector cosine similarity to be high?

### 15.1.6 Scan the QR Code to Discuss<sup>195</sup>



## 15.2 Approximate Training for Word2vec

Recall content of the last section. The core feature of the skip-gram model is the use of softmax operations to compute the conditional probability of generating context word  $w_o$  based on the given central target word  $w_c$ .

$$\mathbb{P}(w_o | w_c) = \frac{\exp(\mathbf{u}_o^\top \mathbf{v}_c)}{\sum_{i \in \mathcal{V}} \exp(\mathbf{u}_i^\top \mathbf{v}_c)}. \quad (15.2.1)$$

<sup>195</sup> <https://discuss.mxnet.io/t/2385>

The logarithmic loss corresponding to the conditional probability is given as

$$-\log \mathbb{P}(w_o | w_c) = -\mathbf{u}_o^\top \mathbf{v}_c + \log \left( \sum_{i \in \mathcal{V}} \exp(\mathbf{u}_i^\top \mathbf{v}_c) \right). \quad (15.2.2)$$

Because the softmax operation has considered that the context word could be any word in the dictionary  $\mathcal{V}$ , the loss mentioned above actually includes the sum of the number of items in the dictionary size. From the last section, we know that for both the skip-gram model and CBOW model, because they both get the conditional probability using a softmax operation, the gradient computation for each step contains the sum of the number of items in the dictionary size. For larger dictionaries with hundreds of thousands or even millions of words, the overhead for computing each gradient may be too high. In order to reduce such computational complexity, we will introduce two approximate training methods in this section: negative sampling and hierarchical softmax. Since there is no major difference between the skip-gram model and the CBOW model, we will only use the skip-gram model as an example to introduce these two training methods in this section.

### 15.2.1 Negative Sampling

Negative sampling modifies the original objective function. Given a context window for the central target word  $w_c$ , we will treat it as an event for context word  $w_o$  to appear in the context window and compute the probability of this event from

$$\mathbb{P}(D = 1 | w_c, w_o) = \sigma(\mathbf{u}_o^\top \mathbf{v}_c), \quad (15.2.3)$$

Here, the  $\sigma$  function has the same definition as the sigmoid activation function:

$$\sigma(x) = \frac{1}{1 + \exp(-x)}. \quad (15.2.4)$$

We will first consider training the word vector by maximizing the joint probability of all events in the text sequence. Given a text sequence of length  $T$ , we assume that the word at time step  $t$  is  $w^{(t)}$  and the context window size is  $m$ . Now we consider maximizing the joint probability

$$\prod_{t=1}^T \prod_{-m \leq j \leq m, j \neq 0} \mathbb{P}(D = 1 | w^{(t)}, w^{(t+j)}). \quad (15.2.5)$$

However, the events included in the model only consider positive examples. In this case, only when all the word vectors are equal and their values approach infinity can the joint probability above be maximized to 1. Obviously, such word vectors are meaningless. Negative sampling makes the objective function more meaningful by sampling with an addition of negative examples. Assume that event  $P$  occurs when context word  $w_o$  appears in the context window of central target word  $w_c$ , and we sample  $K$  words that do not appear in the context window according to the distribution  $\mathbb{P}(w)$  to act as noise words. We assume the event for noise word  $w_k (k = 1, \dots, K)$  to not appear in the context window of central target word  $w_c$  is  $N_k$ . Suppose that events  $P$  and  $N_1, \dots, N_K$  for both positive and negative examples are independent of each other. By considering negative sampling, we can rewrite the joint probability above, which only considers the positive examples, as

$$\prod_{t=1}^T \prod_{-m \leq j \leq m, j \neq 0} \mathbb{P}(w^{(t+j)} | w^{(t)}), \quad (15.2.6)$$

Here, the conditional probability is approximated to be

$$\mathbb{P}(w^{(t+j)} | w^{(t)}) = \mathbb{P}(D = 1 | w^{(t)}, w^{(t+j)}) \prod_{k=1, w_k \sim \mathbb{P}(w)}^K \mathbb{P}(D = 0 | w^{(t)}, w_k). \quad (15.2.7)$$

Let the text sequence index of word  $w^{(t)}$  at time step  $t$  be  $i_t$  and  $h_k$  for noise word  $w_k$  in the dictionary. The logarithmic loss for the conditional probability above is

$$\begin{aligned} -\log \mathbb{P}(w^{(t+j)} | w^{(t)}) &= -\log \mathbb{P}(D = 1 | w^{(t)}, w^{(t+j)}) - \sum_{k=1, w_k \sim \mathbb{P}(w)}^K \log \mathbb{P}(D = 0 | w^{(t)}, w_k) \\ &= -\log \sigma(\mathbf{u}_{i_{t+j}}^\top \mathbf{v}_{i_t}) - \sum_{k=1, w_k \sim \mathbb{P}(w)}^K \log (1 - \sigma(\mathbf{u}_{h_k}^\top \mathbf{v}_{i_t})) \\ &= -\log \sigma(\mathbf{u}_{i_{t+j}}^\top \mathbf{v}_{i_t}) - \sum_{k=1, w_k \sim \mathbb{P}(w)}^K \log \sigma(-\mathbf{u}_{h_k}^\top \mathbf{v}_{i_t}). \end{aligned} \quad (15.2.8)$$

Here, the gradient computation in each step of the training is no longer related to the dictionary size, but linearly related to  $K$ . When  $K$  takes a smaller constant, the negative sampling has a lower computational overhead for each step.

### 15.2.2 Hierarchical Softmax

Hierarchical softmax is another type of approximate training method. It uses a binary tree for data structure, with the leaf nodes of the tree representing every word in the dictionary  $\mathcal{V}$ .

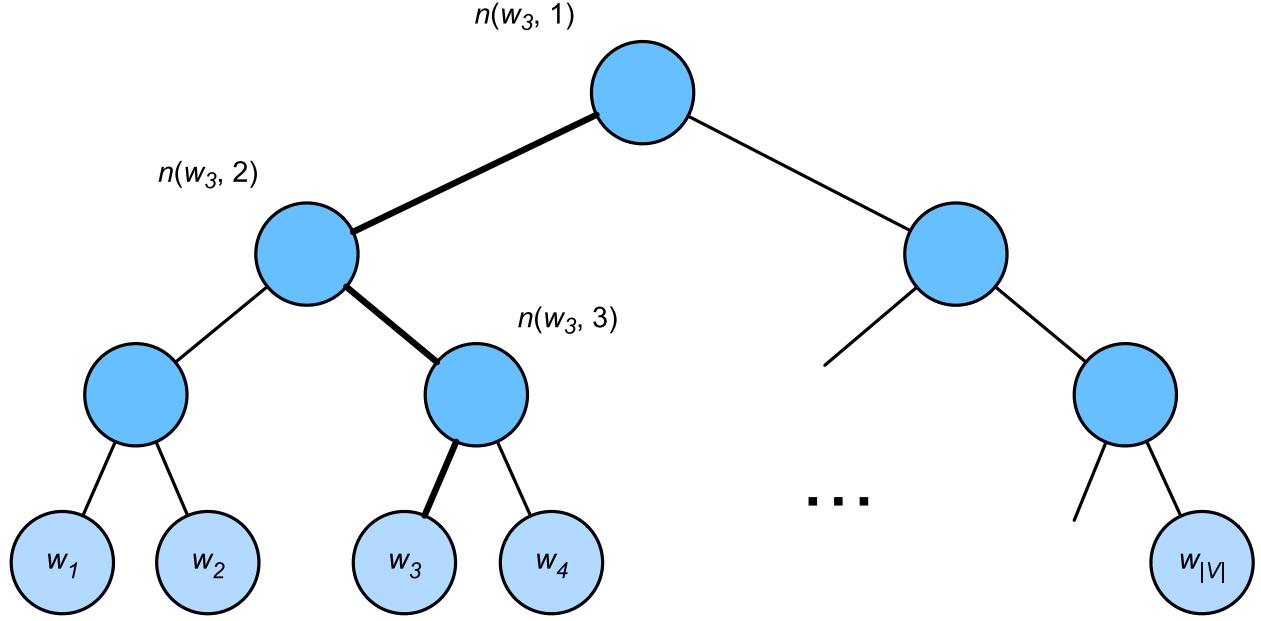


Fig. 15.2.1: Hierarchical Softmax. Each leaf node of the tree represents a word in the dictionary.

We assume that  $L(w)$  is the number of nodes on the path (including the root and leaf nodes) from the root node of the binary tree to the leaf node of word  $w$ . Let  $n(w, j)$  be the  $j$ th node on this path, with the context word vector  $\mathbf{u}_{n(w,j)}$ . We use Figure 12.3 as an example, so  $L(w_3) = 4$ . Hierarchical softmax will approximate the conditional probability in the skip-gram model as

$$\mathbb{P}(w_o | w_c) = \prod_{j=1}^{L(w_o)-1} \sigma([\![n(w_o, j+1) = \text{leftChild}(n(w_o, j))]\!] \cdot \mathbf{u}_{n(w_o, j)}^\top \mathbf{v}_c), \quad (15.2.9)$$

Here the  $\sigma$  function has the same definition as the sigmoid activation function, and  $\text{leftChild}(n)$  is the left child node of node  $n$ . If  $x$  is true,  $[\![x]\!] = 1$ ; otherwise  $[\![x]\!] = -1$ . Now, we will compute the conditional

probability of generating word  $w_3$  based on the given word  $w_c$  in Figure 12.3. We need to find the inner product of word vector  $\mathbf{v}_c$  (for word  $w_c$ ) and each non-leaf node vector on the path from the root node to  $w_3$ . Because, in the binary tree, the path from the root node to leaf node  $w_3$  needs to be traversed left, right, and left again (the path with the bold line in Figure 12.3), we get

$$\mathbb{P}(w_3 | w_c) = \sigma(\mathbf{u}_{n(w_3,1)}^\top \mathbf{v}_c) \cdot \sigma(-\mathbf{u}_{n(w_3,2)}^\top \mathbf{v}_c) \cdot \sigma(\mathbf{u}_{n(w_3,3)}^\top \mathbf{v}_c). \quad (15.2.10)$$

Because  $\sigma(x) + \sigma(-x) = 1$ , the condition that the sum of the conditional probability of any word generated based on the given central target word  $w_c$  in dictionary  $\mathcal{V}$  be 1 will also suffice:

$$\sum_{w \in \mathcal{V}} \mathbb{P}(w | w_c) = 1. \quad (15.2.11)$$

In addition, because the order of magnitude for  $L(w_o) - 1$  is  $\mathcal{O}(\log_2 |\mathcal{V}|)$ , when the size of dictionary  $\mathcal{V}$  is large, the computational overhead for each step in the hierarchical softmax training is greatly reduced compared to situations where we do not use approximate training.

### 15.2.3 Summary

- Negative sampling constructs the loss function by considering independent events that contain both positive and negative examples. The gradient computational overhead for each step in the training process is linearly related to the number of noise words we sample.
- Hierarchical softmax uses a binary tree and constructs the loss function based on the path from the root node to the leaf node. The gradient computational overhead for each step in the training process is related to the logarithm of the dictionary size.

### 15.2.4 Exercises

- Before reading the next section, think about how we should sample noise words in negative sampling.
- What makes the last formula in this section hold?
- How can we apply negative sampling and hierarchical softmax in the skip-gram model?

### 15.2.5 Scan the QR Code to Discuss<sup>196</sup>



## 15.3 Data Sets for Word2vec

In this section, we will introduce how to preprocess a data set with negative sampling Section 15.2 and load into mini-batches for word2vec training. The data set we use is Penn Tree Bank (PTB)<sup>197</sup>, which is a small

<sup>196</sup> <https://discuss.mxnet.io/t/2386>

<sup>197</sup> <https://catalog.ldc.upenn.edu/LDC99T42>

but commonly-used corpus. It takes samples from Wall Street Journal articles and includes training sets, validation sets, and test sets.

First, import the packages and modules required for the experiment.

```
import collections
import d2l
import math
from mxnet import nd, gluon
import random
import zipfile
```

### 15.3.1 Read and Preprocessing

This data set has already been preprocessed. Each line of the data set acts as a sentence. All the words in a sentence are separated by spaces. In the word embedding task, each word is a token.

```
# Save to the d2l package.
def read_ptb():
    with zipfile.ZipFile('../data/ptb.zip', 'r') as f:
        raw_text = f.read('ptb/ptb.train.txt').decode("utf-8")
    return [line.split() for line in raw_text.split('\n')]

sentences = read_ptb()
'# sentences: %d' % len(sentences)
```

```
'# sentences: 42069'
```

Next we build a vocabulary with words appeared not greater than 10 times mapped into a “<unk>” token. Note that the preprocessed PTB data also contains “<unk>” tokens presenting rare words.

```
vocab = d2l.Vocab(sentences, min_freq=10)
'vocab size: %d' % len(vocab)
```

```
'vocab size: 6719'
```

### 15.3.2 Subsampling

In text data, there are generally some words that appear at high frequencies, such as “the”, “a”, and “in” in English. Generally speaking, in a context window, it is better to train the word embedding model when a word (such as “chip”) and a lower-frequency word (such as “microprocessor”) appear at the same time, rather than when a word appears with a higher-frequency word (such as “the”). Therefore, when training the word embedding model, we can perform subsampling[2] on the words. Specifically, each indexed word  $w_i$  in the data set will drop out at a certain probability. The dropout probability is given as:

$$\mathbb{P}(w_i) = \max \left( 1 - \sqrt{\frac{t}{f(w_i)}}, 0 \right), \quad (15.3.1)$$

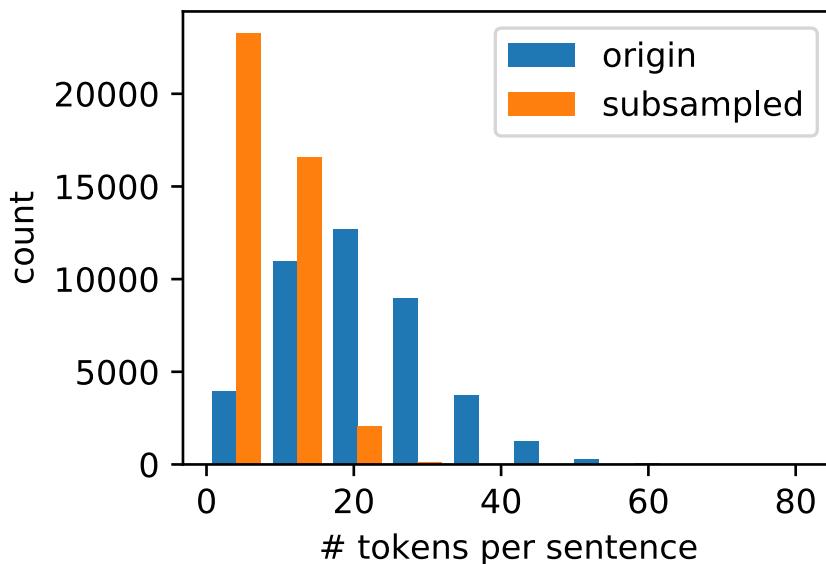
Here,  $f(w_i)$  is the ratio of the instances of word  $w_i$  to the total number of words in the data set, and the constant  $t$  is a hyper-parameter (set to  $10^{-4}$  in this experiment). As we can see, it is only possible to drop out the word  $w_i$  in subsampling when  $f(w_i) > t$ . The higher the word’s frequency, the higher its dropout probability.

```
# Save to the d2l package.
def subsampling(sentences, vocab):
    # Map low frequency words into <unk>
    sentences = [[vocab.idx_to_token[vocab[tk]] for tk in line]
                  for line in sentences]
    # Count the frequency for each word
    counter = d2l.count_corpus(sentences)
    num_tokens = sum(counter.values())
    # Return True if to keep this token during subsampling
    keep = lambda token: (
        random.uniform(0, 1) < math.sqrt(1e-4 / counter[token] * num_tokens))
    # Now do the subsampling.
    return [[tk for tk in line if keep(tk)] for line in sentences]

subsampled = subsampling(sentences, vocab)
```

Compare the sequence lengths before and after sampling, we can see subsampling significantly reduced the sequence length.

```
d2l.set_figsize((3.5, 2.5))
d2l.plt.hist([[len(line) for line in sentences],
              [len(line) for line in subsampled]])
d2l.plt.xlabel('# tokens per sentence')
d2l.plt.ylabel('count')
d2l.plt.legend(['origin', 'subsampled']);
```



For individual tokens, the sampling rate of the high-frequency word “the” is less than 1/20.

```
def compare_counts(token):
    return '# of "%s": before=%d, after=%d' % (token, sum(
        [line.count(token) for line in sentences]), sum(
        [line.count(token) for line in subsampled]))

compare_counts('the')
```

```
'# of "the": before=50770, after=2138'
```

But the low-frequency word “join” is completely preserved.

```
compare_counts('join')
```

```
'# of "join": before=45, after=45'
```

Lastly, we map each token into an index to construct the corpus.

```
corpus = [vocab[line] for line in subsampled]
corpus[0:3]
```

```
[[0, 0], [2, 32, 2132, 145, 406], [140, 3, 5464, 3080, 1595]]
```

### 15.3.3 Load the Data Set

Next we read the corpus with token indices into data batches for training.

#### Extract Central Target Words and Context Words

We use words with a distance from the central target word not exceeding the context window size as the context words of the given center target word. The following definition function extracts all the central target words and their context words. It uniformly and randomly samples an integer to be used as the context window size between integer 1 and the `max_window_size` (maximum context window).

```
# Save to the d2l package.
def get_centers_and_contexts(corpus, max_window_size):
    centers, contexts = [], []
    for line in corpus:
        # Each sentence needs at least 2 words to form a
        # "central target word - context word" pair
        if len(line) < 2: continue
        centers += line
        for i in range(len(line)): # Context window centered at i
            window_size = random.randint(1, max_window_size)
            indices = list(range(max(0, i - window_size),
                                 min(len(line), i + 1 + window_size)))
            # Exclude the central target word from the context words
            indices.remove(i)
            contexts.append([line[idx] for idx in indices])
    return centers, contexts
```

Next, we create an artificial data set containing two sentences of 7 and 3 words, respectively. Assume the maximum context window is 2 and print all the central target words and their context words.

```
tiny_dataset = [list(range(7)), list(range(7, 10))]
print('dataset', tiny_dataset)
for center, context in zip(*get_centers_and_contexts(tiny_dataset, 2)):
    print('center', center, 'has contexts', context)
```

```
dataset [[0, 1, 2, 3, 4, 5, 6], [7, 8, 9]]
center 0 has contexts [1]
center 1 has contexts [0, 2, 3]
center 2 has contexts [0, 1, 3, 4]
center 3 has contexts [1, 2, 4, 5]
center 4 has contexts [3, 5]
center 5 has contexts [3, 4, 6]
center 6 has contexts [5]
center 7 has contexts [8]
center 8 has contexts [7, 9]
center 9 has contexts [8]
```

We set the maximum context window size to 5. The following extracts all the central target words and their context words in the data set.

```
all_centers, all_contexts = get_centers_and_contexts(corpus, 5)
'# center-context pairs: %d' % len(all_centers)

'# center-context pairs: 352743'
```

## Negative Sampling

We use negative sampling for approximate training. For a central and context word pair, we randomly sample  $K$  noise words ( $K = 5$  in the experiment). According to the suggestion in the Word2vec paper, the noise word sampling probability  $\mathbb{P}(w)$  is the ratio of the word frequency of  $w$  to the total word frequency raised to the power of 0.75 [2].

We first define a class to draw a candidate according to the sampling weights. It caches a 10000 size random number bank instead of calling `random.choices` every time.

```
# Save to the d2l package.
class RandomGenerator(object):
    """Draw a random int in [0, n] according to n sampling weights"""
    def __init__(self, sampling_weights):
        self.population = list(range(len(sampling_weights)))
        self.sampling_weights = sampling_weights
        self.candidates = []
        self.i = 0

    def draw(self):
        if self.i == len(self.candidates):
            self.candidates = random.choices(
                self.population, self.sampling_weights, k=10000)
            self.i = 0
        self.i += 1
        return self.candidates[self.i-1]

generator = RandomGenerator([2,3,4])
[generator.draw() for _ in range(10)]
```

```
[2, 2, 1, 2, 2, 1, 2, 2, 1, 0]
```

```
# Save to the d2l package.
def get_negatives(all_contexts, corpus, K):
    counter = d2l.count_corpus(corpus)
    sampling_weights = [counter[i]**0.75 for i in range(len(counter))]
    all_negatives, generator = [], RandomGenerator(sampling_weights)
    for contexts in all_contexts:
        negatives = []
        while len(negatives) < len(contexts) * K:
            neg = generator.draw()
            # Noise words cannot be context words
            if neg not in contexts:
                negatives.append(neg)
        all_negatives.append(negatives)
    return all_negatives

all_negatives = get_negatives(all_contexts, corpus, 5)
```

### Read into Batches

We extract all central target words `all_centers`, and the context words `all_contexts` and noise words `all_negatives` of each central target word from the data set. We will read them in random mini-batches.

In a mini-batch of data, the  $i$ -th example includes a central word and its corresponding  $n_i$  context words and  $m_i$  noise words. Since the context window size of each example may be different, the sum of context words and noise words,  $n_i + m_i$ , will be different. When constructing a mini-batch, we concatenate the context words and noise words of each example, and add 0s for padding until the length of the concatenations are the same, that is, the length of all concatenations is  $\max_i n_i + m_i$  (`max_len`). In order to avoid the effect of padding on the loss function calculation, we construct the mask variable `masks`, each element of which corresponds to an element in the concatenation of context and noise words, `contexts_negatives`. When an element in the variable `contexts_negatives` is a padding, the element in the mask variable `masks` at the same position will be 0. Otherwise, it takes the value 1. In order to distinguish between positive and negative examples, we also need to distinguish the context words from the noise words in the `contexts_negatives` variable. Based on the construction of the mask variable, we only need to create a label variable `labels` with the same shape as the `contexts_negatives` variable and set the elements corresponding to context words (positive examples) to 1, and the rest to 0.

Next, we will implement the mini-batch reading function `batchify`. Its mini-batch input `data` is a list whose length is the batch size, each element of which contains central target words `center`, context words `context`, and noise words `negative`. The mini-batch data returned by this function conforms to the format we need, for example, it includes the mask variable.

```
# Save to the d2l package.
def batchify(data):
    max_len = max(len(c) + len(n) for _, c, n in data)
    centers, contexts_negatives, masks, labels = [], [], [], []
    for center, context, negative in data:
        cur_len = len(context) + len(negative)
        centers += [center]
        contexts_negatives += [context + negative + [0] * (max_len - cur_len)]
        masks += [[1] * cur_len + [0] * (max_len - cur_len)]
        labels += [[1] * len(context) + [0] * (max_len - len(context))]

    return (nd.array(centers).reshape((-1, 1)), nd.array(contexts_negatives),
            nd.array(masks), nd.array(labels))
```

Construct two simple examples:

```
x_1 = ([1, [2,2], [3,3,3,3])
x_2 = ([1, [2,2,2], [3,3])
batch = batchify((x_1, x_2))

names = ['centers', 'contexts_negatives', 'masks', 'labels']
for name, data in zip(names, batch):
    print(name, '=', data)
```

```
centers =
[[1.]
 [1.]]
<NDArray 2x1 @cpu(0)>
contexts_negatives =
[[2. 2. 3. 3. 3. 3.]
 [2. 2. 2. 3. 3. 0.]]
<NDArray 2x6 @cpu(0)>
masks =
[[1. 1. 1. 1. 1. 1.]
 [1. 1. 1. 1. 1. 0.]]
<NDArray 2x6 @cpu(0)>
labels =
[[1. 1. 0. 0. 0. 0.]
 [1. 1. 1. 0. 0. 0.]]
<NDArray 2x6 @cpu(0)>
```

We use the `batchify` function just defined to specify the mini-batch reading method in the `DataLoader` instance.

### 15.3.4 Put All Things Together

Lastly, we define the `load_data_ptb` function that read the PTB data set and return the data loader.

```
# Save to the d2l package.
def load_data_ptb(batch_size, max_window_size, num_noise_words):
    sentences = read_ptb()
    vocab = d2l.Vocab(sentences, min_freq=10)
    subsampled = subsampling(sentences, vocab)
    corpus = [vocab[line] for line in subsampled]
    all_centers, all_contexts = get_centers_and_contexts(
        corpus, max_window_size)
    all_negatives = get_negatives(all_contexts, corpus, num_noise_words)
    dataset = gluon.data.ArrayDataset(
        all_centers, all_contexts, all_negatives)
    data_iter = gluon.data.DataLoader(dataset, batch_size, shuffle=True,
                                      batchify_fn=batchify)
    return data_iter, vocab
```

Let's print the first mini-batch of the data iterator.

```
data_iter, vocab = load_data_ptb(512, 5, 5)
for batch in data_iter:
```

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```
for name, data in zip(names, batch):
    print(name, 'shape:', data.shape)
break
```

```
centers shape: (512, 1)
contexts_negatives shape: (512, 60)
masks shape: (512, 60)
labels shape: (512, 60)
```

### 15.3.5 Summary

- Subsampling attempts to minimize the impact of high-frequency words on the training of a word embedding model.
- We can pad examples of different lengths to create mini-batches with examples of all the same length and use mask variables to distinguish between padding and non-padding elements, so that only non-padding elements participate in the calculation of the loss function.

### 15.3.6 Exercises

- We use the `batchify` function to specify the mini-batch reading method in the `DataLoader` instance and print the shape of each variable in the first batch read. How should these shapes be calculated?

## 15.4 Implementation of Word2vec

In this section, we will train a skip-gram model defined in Section 15.1.

First, import the packages and modules required for the experiment, and load the PTB data set.

```
import d2l
from mxnet import autograd, gluon, nd
from mxnet.gluon import nn

batch_size, max_window_size, num_noise_words = 512, 5, 5
data_iter, vocab = d2l.load_data_ptb(512, 5, 5)
```

### 15.4.1 The Skip-Gram Model

We will implement the skip-gram model by using embedding layers and mini-batch multiplication. These methods are also often used to implement other natural language processing applications.

#### Embedding Layer

The layer in which the obtained word is embedded is called the embedding layer, which can be obtained by creating an `nn.Embedding` instance in Gluon. The weight of the embedding layer is a matrix whose number of rows is the dictionary size (`input_dim`) and whose number of columns is the dimension of each word vector (`output_dim`). We set the dictionary size to 20 and the word vector dimension to 4.

```
embed = nn.Embedding(input_dim=20, output_dim=4)
embed.initialize()
embed.weight
```

```
Parameter embedding0_weight (shape=(20, 4), dtype=float32)
```

The input of the embedding layer is the index of the word. When we enter the index  $i$  of a word, the embedding layer returns the  $i$ th row of the weight matrix as its word vector. Below we enter an index of shape (2,3) into the embedding layer. Because the dimension of the word vector is 4, we obtain a word vector of shape (2,3,4).

```
x = nd.array([[1, 2, 3], [4, 5, 6]])
embed(x)
```

```
[[[ 0.01438687  0.05011239  0.00628365  0.04861524]
[-0.01068833  0.01729892  0.02042518 -0.01618656]
[-0.00873779 -0.02834515  0.05484822 -0.06206018]]

[[ 0.06491279 -0.03182812 -0.01631819 -0.00312688]
[ 0.0408415   0.04370362  0.00404529 -0.0028032 ]
[ 0.00952624 -0.01501013  0.05958354  0.04705103]]]
<NDArray 2x3x4 @cpu(0)>
```

### Mini-batch Multiplication

We can multiply the matrices in two mini-batches one by one, by the mini-batch multiplication operation `batch_dot`. Suppose the first batch contains  $n$  matrices  $\mathbf{X}_1, \dots, \mathbf{X}_n$  with a shape of  $a \times b$ , and the second batch contains  $n$  matrices  $\mathbf{Y}_1, \dots, \mathbf{Y}_n$  with a shape of  $b \times c$ . The output of matrix multiplication on these two batches are  $n$  matrices  $\mathbf{X}_1\mathbf{Y}_1, \dots, \mathbf{X}_n\mathbf{Y}_n$  with a shape of  $a \times c$ . Therefore, given two NDArrays of shape  $(n, a, b)$  and  $(n, b, c)$ , the shape of the mini-batch multiplication output is  $(n, a, c)$ .

```
X = nd.ones((2, 1, 4))
Y = nd.ones((2, 4, 6))
nd.batch_dot(X, Y).shape
```

```
(2, 1, 6)
```

### Skip-gram Model Forward Calculation

In forward calculation, the input of the skip-gram model contains the central target word index `center` and the concatenated context and noise word index `contexts_and_negatives`. In which, the `center` variable has the shape (batch size, 1), while the `contexts_and_negatives` variable has the shape (batch size, `max_len`). These two variables are first transformed from word indexes to word vectors by the word embedding layer, and then the output of shape (batch size, 1, `max_len`) is obtained by mini-batch multiplication. Each element in the output is the inner product of the central target word vector and the context word vector or noise word vector.

```
def skip_gram(center, contexts_and_negatives, embed_v, embed_u):
    v = embed_v(center)
    u = embed_u(contexts_and_negatives)
```

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```
pred = nd.batch_dot(v, u.swapaxes(1, 2))
return pred
```

Verify that the output shape should be (batch size, 1, max\_len).

```
skip_gram(nd.ones((2,1)), nd.ones((2,4)), embed, embed).shape
```

```
(2, 1, 4)
```

## 15.4.2 Training

Before training the word embedding model, we need to define the loss function of the model.

### Binary Cross Entropy Loss Function

According to the definition of the loss function in negative sampling, we can directly use Gluon's binary cross-entropy loss function `SigmoidBinaryCrossEntropyLoss`.

```
loss = gluon.loss.SigmoidBinaryCrossEntropyLoss()
```

It is worth mentioning that we can use the mask variable to specify the partial predicted value and label that participate in loss function calculation in the mini-batch: when the mask is 1, the predicted value and label of the corresponding position will participate in the calculation of the loss function; When the mask is 0, the predicted value and label of the corresponding position do not participate in the calculation of the loss function. As we mentioned earlier, mask variables can be used to avoid the effect of padding on loss function calculations.

Given two identical examples, different masks lead to different loss values.

```
pred = nd.array([[.5]*4]*2)
label = nd.array([[1,0,1,0]]*2)
mask = nd.array([[1, 1, 1, 1], [1, 1, 0, 0]])
loss(pred, label, mask)
```

```
[0.724077 0.3620385]
<NDArray 2 @cpu(0)>
```

We can normalize the loss in each example due to various lengths in each example.

```
loss(pred, label, mask) / mask.sum(axis=1) * mask.shape[1]
```

```
[0.724077 0.724077]
<NDArray 2 @cpu(0)>
```

### Initialize Model Parameters

We construct the embedding layers of the central and context words, respectively, and set the hyper-parameter word vector dimension `embed_size` to 100.

```
embed_size = 100
net = nn.Sequential()
net.add(nn.Embedding(input_dim=len(vocab), output_dim=embed_size),
        nn.Embedding(input_dim=len(vocab), output_dim=embed_size))
```

## Training

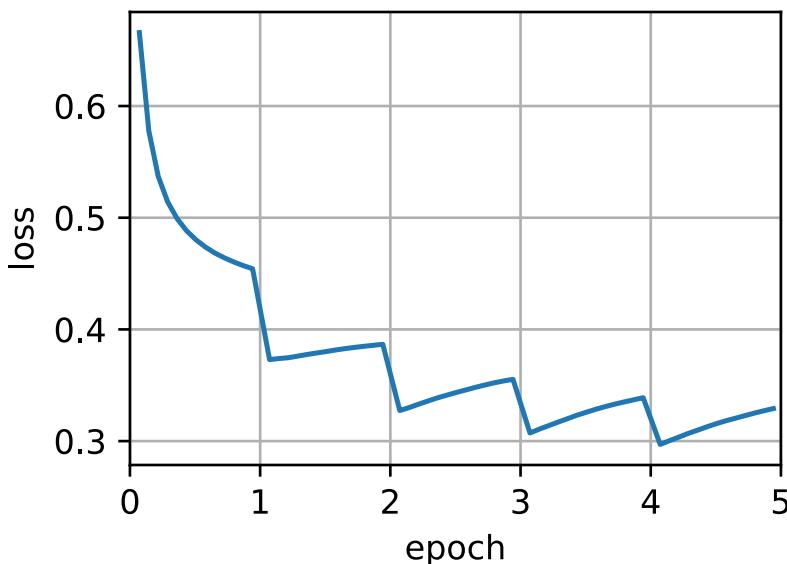
The training function is defined below. Because of the existence of padding, the calculation of the loss function is slightly different compared to the previous training functions.

```
def train(net, data_iter, lr, num_epochs, ctx=d2l.try_gpu()):
    net.initialize(ctx=ctx, force_reinit=True)
    trainer = gluon.Trainer(net.collect_params(), 'adam',
                           {'learning_rate': lr})
    animator = d2l.Animator(xlabel='epoch', ylabel='loss',
                           xlim=[0, num_epochs])
    for epoch in range(num_epochs):
        timer = d2l.Timer()
        metric = d2l.Accumulator(2) # loss_sum, num_tokens
        for i, batch in enumerate(data_iter):
            center, context_negative, mask, label = [
                data.as_in_context(ctx) for data in batch]
            with autograd.record():
                pred = skip_gram(center, context_negative, net[0], net[1])
                l = (loss(pred.reshape(label.shape), label, mask)
                     / mask.sum(axis=1) * mask.shape[1])
            l.backward()
            trainer.step(batch_size)
            metric.add(l.sum().asscalar(), l.size)
            if (i+1) % 50 == 0:
                animator.add(epoch+(i+1)/len(data_iter), metric[0]/metric[1])
        print('loss %.3f, %d tokens/sec on %s' %
              (metric[0]/metric[1], metric[1]/timer.stop(), ctx))
```

Now, we can train a skip-gram model using negative sampling.

```
lr, num_epochs = 0.01, 5
train(net, data_iter, lr, num_epochs)
```

```
loss 0.331, 15756 tokens/sec on gpu(0)
```



### 15.4.3 Applying the Word Embedding Model

After training the word embedding model, we can represent similarity in meaning between words based on the cosine similarity of two word vectors. As we can see, when using the trained word embedding model, the words closest in meaning to the word “chip” are mostly related to chips.

```
def get_similar_tokens(query_token, k, embed):
    W = embed.weight.data()
    x = W[vocab[query_token]]
    # Compute the cosine similarity. Add 1e-9 for numerical stability.
    cos = nd.dot(W, x) / (nd.sum(W * W, axis=1) * nd.sum(x * x) + 1e-9).sqrt()
    topk = nd.topk(cos, k=k+1, ret_typ='indices').asnumpy().astype('int32')
    for i in topk[1:]: # Remove the input words
        print('cosine sim=% .3f: %s' % (cos[i].asscalar(), (vocab.idx_to_token[i])))

get_similar_tokens('chip', 3, net[0])
```

```
cosine sim=0.557: microprocessor
cosine sim=0.525: intel
cosine sim=0.449: ibm
```

### 15.4.4 Summary

- We can use Gluon to train a skip-gram model through negative sampling.

### 15.4.5 Exercises

- Set `sparse_grad=True` when creating an instance of `nn.Embedding`. Does it accelerate training? Look up MXNet documentation to learn the meaning of this argument.
- Try to find synonyms for other words.

- Tune the hyper-parameters and observe and analyze the experimental results.
- When the data set is large, we usually sample the context words and the noise words for the central target word in the current mini-batch only when updating the model parameters. In other words, the same central target word may have different context words or noise words in different epochs. What are the benefits of this sort of training? Try to implement this training method.

#### 15.4.6 Scan the QR Code to Discuss<sup>198</sup>



## 15.5 Subword Embedding (fastText)

English words usually have internal structures and formation methods. For example, we can deduce the relationship between “dog”, “dogs”, and “dogcatcher” by their spelling. All these words have the same root, “dog”, but they use different suffixes to change the meaning of the word. Moreover, this association can be extended to other words. For example, the relationship between “dog” and “dogs” is just like the relationship between “cat” and “cats”. The relationship between “boy” and “boyfriend” is just like the relationship between “girl” and “girlfriend”. This characteristic is not unique to English. In French and Spanish, a lot of verbs can have more than 40 different forms depending on the context. In Finnish, a noun may have more than 15 forms. In fact, morphology, which is an important branch of linguistics, studies the internal structure and formation of words.

In word2vec, we did not directly use morphology information. In both the skip-gram model and continuous bag-of-words model, we use different vectors to represent words with different forms. For example, “dog” and “dogs” are represented by two different vectors, while the relationship between these two vectors is not directly represented in the model. In view of this, fastText [4] proposes the method of subword embedding, thereby attempting to introduce morphological information in the skip-gram model in word2vec.

In fastText, each central word is represented as a collection of subwords. Below we use the word “where” as an example to understand how subwords are formed. First, we add the special characters “<” and “>” at the beginning and end of the word to distinguish the subwords used as prefixes and suffixes. Then, we treat the word as a sequence of characters to extract the  $n$ -grams. For example, when  $n = 3$ , we can get all subwords with a length of 3:

$$\text{"<wh", "whe", "her", "ere", "re>"}, \quad (15.5.1)$$

and the special subword “<where>”.

In fastText, for a word  $w$ , we record the union of all its subwords with length of 3 to 6 and special subwords as  $\mathcal{G}_w$ . Thus, the dictionary is the union of the collection of subwords of all words. Assume the vector of the subword  $g$  in the dictionary is  $\mathbf{z}_g$ . Then, the central word vector  $\mathbf{u}_w$  for the word  $w$  in the skip-gram model can be expressed as

$$\mathbf{u}_w = \sum_{g \in \mathcal{G}_w} \mathbf{z}_g. \quad (15.5.2)$$

---

<sup>198</sup> <https://discuss.mxnet.io/t/2387>

The rest of the fastText process is consistent with the skip-gram model, so it is not repeated here. As we can see, compared with the skip-gram model, the dictionary in fastText is larger, resulting in more model parameters. Also, the vector of one word requires the summation of all subword vectors, which results in higher computation complexity. However, we can obtain better vectors for more uncommon complex words, even words not existing in the dictionary, by looking at other words with similar structures.

### 15.5.1 Summary

- FastText proposes a subword embedding method. Based on the skip-gram model in word2vec, it represents the central word vector as the sum of the subword vectors of the word.
- Subword embedding utilizes the principles of morphology, which usually improves the quality of representations of uncommon words.

### 15.5.2 Exercises

- When there are too many subwords (for example, 6 words in English result in about  $3 \times 10^8$  combinations), what problems arise? Can you think of any methods to solve them? Hint: Refer to the end of section 3.2 of the fastText paper[1].
- How can you design a subword embedding model based on the continuous bag-of-words model?

### 15.5.3 Scan the QR Code to Discuss<sup>199</sup>



## 15.6 Word Embedding with Global Vectors (GloVe)

First, we should review the skip-gram model in word2vec. The conditional probability  $\mathbb{P}(w_j | w_i)$  expressed in the skip-gram model using the softmax operation will be recorded as  $q_{ij}$ , that is:

$$q_{ij} = \frac{\exp(\mathbf{u}_j^\top \mathbf{v}_i)}{\sum_{k \in \mathcal{V}} \exp(\mathbf{u}_k^\top \mathbf{v}_i)}, \quad (15.6.1)$$

where  $\mathbf{v}_i$  and  $\mathbf{u}_i$  are the vector representations of word  $w_i$  of index  $i$  as the center word and context word respectively, and  $\mathcal{V} = \{0, 1, \dots, |\mathcal{V}| - 1\}$  is the vocabulary index set.

For word  $w_i$ , it may appear in the data set for multiple times. We collect all the context words every time when  $w_i$  is a center word and keep duplicates, denoted as multiset  $\mathcal{C}_i$ . The number of an element in a multiset is called the multiplicity of the element. For instance, suppose that word  $w_i$  appears twice in the data set: the context windows when these two  $w_i$  become center words in the text sequence contain context word indices 2, 1, 5, 2 and 2, 3, 2, 1. Then, multiset  $\mathcal{C}_i = \{1, 1, 2, 2, 2, 2, 3, 5\}$ , where multiplicity of element 1 is 2, multiplicity of element 2 is 4, and multiplicities of elements 3 and 5 are both 1. Denote multiplicity of element  $j$  in multiset  $\mathcal{C}_i$  as  $x_{ij}$ : it is the number of word  $w_j$  in all the context windows for center word  $w_i$ .

<sup>199</sup> <https://discuss.mxnet.io/t/2388>

in the entire data set. As a result, the loss function of the skip-gram model can be expressed in a different way:

$$-\sum_{i \in \mathcal{V}} \sum_{j \in \mathcal{V}} x_{ij} \log q_{ij}. \quad (15.6.2)$$

We add up the number of all the context words for the central target word  $w_i$  to get  $x_i$ , and record the conditional probability  $x_{ij}/x_i$  for generating context word  $w_j$  based on central target word  $w_i$  as  $p_{ij}$ . We can rewrite the loss function of the skip-gram model as

$$-\sum_{i \in \mathcal{V}} x_i \sum_{j \in \mathcal{V}} p_{ij} \log q_{ij}. \quad (15.6.3)$$

In the formula above,  $\sum_{j \in \mathcal{V}} p_{ij} \log q_{ij}$  computes the conditional probability distribution  $p_{ij}$  for context word generation based on the central target word  $w_i$  and the cross-entropy of conditional probability distribution  $q_{ij}$  predicted by the model. The loss function is weighted using the sum of the number of context words with the central target word  $w_i$ . If we minimize the loss function from the formula above, we will be able to allow the predicted conditional probability distribution to approach as close as possible to the true conditional probability distribution.

However, although the most common type of loss function, the cross-entropy loss function is sometimes not a good choice. On the one hand, as we mentioned in [Section 15.2](#) the cost of letting the model prediction  $q_{ij}$  become the legal probability distribution has the sum of all items in the entire dictionary in its denominator. This can easily lead to excessive computational overhead. On the other hand, there are often a lot of uncommon words in the dictionary, and they appear rarely in the data set. In the cross-entropy loss function, the final prediction of the conditional probability distribution on a large number of uncommon words is likely to be inaccurate.

### 15.6.1 The GloVe Model

To address this, GloVe [48], a word embedding model that came after word2vec, adopts square loss and makes three changes to the skip-gram model based on this loss.

1. Here, we use the non-probability distribution variables  $p'_{ij} = x_{ij}$  and  $q'_{ij} = \exp(\mathbf{u}_j^\top \mathbf{v}_i)$  and take their logs. Therefore, we get the square loss  $(\log p'_{ij} - \log q'_{ij})^2 = (\mathbf{u}_j^\top \mathbf{v}_i - \log x_{ij})^2$ .
2. We add two scalar model parameters for each word  $w_i$ : the bias terms  $b_i$  (for central target words) and  $c_i$  (for context words).
3. Replace the weight of each loss with the function  $h(x_{ij})$ . The weight function  $h(x)$  is a monotone increasing function with the range  $[0,1]$ .

Therefore, the goal of GloVe is to minimize the loss function.

$$\sum_{i \in \mathcal{V}} \sum_{j \in \mathcal{V}} h(x_{ij}) (\mathbf{u}_j^\top \mathbf{v}_i + b_i + c_j - \log x_{ij})^2. \quad (15.6.4)$$

Here, we have a suggestion for the choice of weight function  $h(x)$ : when  $x < c$  (e.g  $c = 100$ ), make  $h(x) = (x/c)^\alpha$  (e.g  $\alpha = 0.75$ ), otherwise make  $h(x) = 1$ . Because  $h(0) = 0$ , the squared loss term for  $x_{ij} = 0$  can be simply ignored. When we use mini-batch SGD for training, we conduct random sampling to get a non-zero mini-batch  $x_{ij}$  from each time step and compute the gradient to update the model parameters. These non-zero  $x_{ij}$  are computed in advance based on the entire data set and they contain global statistics for the data set. Therefore, the name GloVe is taken from “Global Vectors”.

Notice that if word  $w_i$  appears in the context window of word  $w_j$ , then word  $w_j$  will also appear in the context window of word  $w_i$ . Therefore,  $x_{ij} = x_{ji}$ . Unlike word2vec, GloVe fits the symmetric  $\log x_{ij}$  in lieu of the asymmetric conditional probability  $p_{ij}$ . Therefore, the central target word vector and context word

vector of any word are equivalent in GloVe. However, the two sets of word vectors that are learned by the same word may be different in the end due to different initialization values. After learning all the word vectors, GloVe will use the sum of the central target word vector and the context word vector as the final word vector for the word.

### 15.6.2 Understanding GloVe from Conditional Probability Ratios

We can also try to understand GloVe word embedding from another perspective. We will continue the use of symbols from earlier in this section,  $\mathbb{P}(w_j | w_i)$  represents the conditional probability of generating context word  $w_j$  with central target word  $w_i$  in the data set, and it will be recorded as  $p_{ij}$ . From a real example from a large corpus, here we have the following two sets of conditional probabilities with “ice” and “steam” as the central target words and the ratio between them:

$w_k =$	“solid”	“gas”	“water”	“fashion”
$p_1 = \mathbb{P}(w_k   \text{“ice”})$	0.00019	0.000066	0.003	0.000017
$p_2 = \mathbb{P}(w_k   \text{“steam”})$	0.000022	0.00078	0.0022	0.000018
$p_1/p_2$	8.9	0.085	1.36	0.96

We will be able to observe phenomena such as:

- For a word  $w_k$  that is related to “ice” but not to “steam”, such as  $w_k = \text{“solid”}$ , we would expect a larger conditional probability ratio, like the value 8.9 in the last row of the table above.
- For a word  $w_k$  that is related to “steam” but not to “ice”, such as  $w_k = \text{“gas”}$ , we would expect a smaller conditional probability ratio, like the value 0.085 in the last row of the table above.
- For a word  $w_k$  that is related to both “ice” and “steam”, such as  $w_k = \text{“water”}$ , we would expect a conditional probability ratio close to 1, like the value 1.36 in the last row of the table above.
- For a word  $w_k$  that is related to neither “ice” or “steam”, such as  $w_k = \text{“fashion”}$ , we would expect a conditional probability ratio close to 1, like the value 0.96 in the last row of the table above.

We can see that the conditional probability ratio can represent the relationship between different words more intuitively. We can construct a word vector function to fit the conditional probability ratio more effectively. As we know, to obtain any ratio of this type requires three words  $w_i$ ,  $w_j$ , and  $w_k$ . The conditional probability ratio with  $w_i$  as the central target word is  $p_{ij}/p_{ik}$ . We can find a function that uses word vectors to fit this conditional probability ratio.

$$f(\mathbf{u}_j, \mathbf{u}_k, \mathbf{v}_i) \approx \frac{p_{ij}}{p_{ik}}. \quad (15.6.5)$$

The possible design of function  $f$  here will not be unique. We only need to consider a more reasonable possibility. Notice that the conditional probability ratio is a scalar, we can limit  $f$  to be a scalar function:  $f(\mathbf{u}_j, \mathbf{u}_k, \mathbf{v}_i) = f((\mathbf{u}_j - \mathbf{u}_k)^\top \mathbf{v}_i)$ . After exchanging index  $j$  with  $k$ , we will be able to see that function  $f$  satisfies the condition  $f(x)f(-x) = 1$ , so one possibility could be  $f(x) = \exp(x)$ . Thus:

$$f(\mathbf{u}_j, \mathbf{u}_k, \mathbf{v}_i) = \frac{\exp(\mathbf{u}_j^\top \mathbf{v}_i)}{\exp(\mathbf{u}_k^\top \mathbf{v}_i)} \approx \frac{p_{ij}}{p_{ik}}. \quad (15.6.6)$$

One possibility that satisfies the right side of the approximation sign is  $\exp(\mathbf{u}_j^\top \mathbf{v}_i) \approx \alpha p_{ij}$ , where  $\alpha$  is a constant. Considering that  $p_{ij} = x_{ij}/x_i$ , after taking the logarithm we get  $\mathbf{u}_j^\top \mathbf{v}_i \approx \log \alpha + \log x_{ij} - \log x_i$ . We use additional bias terms to fit  $-\log \alpha + \log x_i$ , such as the central target word bias term  $b_i$  and context word bias term  $c_j$ :

$$\mathbf{u}_j^\top \mathbf{v}_i + b_i + c_j \approx \log(x_{ij}). \quad (15.6.7)$$

By taking the square error and weighting the left and right sides of the formula above, we can get the loss function of GloVe.

### 15.6.3 Summary

- In some cases, the cross-entropy loss function may have a disadvantage. GloVe uses squared loss and the word vector to fit global statistics computed in advance based on the entire data set.
- The central target word vector and context word vector of any word are equivalent in GloVe.

### 15.6.4 Exercises

- If a word appears in the context window of another word, how can we use the distance between them in the text sequence to redesign the method for computing the conditional probability  $p_{ij}$ ? Hint: See section 4.2 from the paper GloVe [48].
- For any word, will its central target word bias term and context word bias term be equivalent to each other in GloVe? Why?

### 15.6.5 Scan the QR Code to Discuss<sup>200</sup>



## 15.7 Finding Synonyms and Analogies

In Section 15.4 we trained a word2vec word embedding model on a small-scale data set and searched for synonyms using the cosine similarity of word vectors. In practice, word vectors pre-trained on a large-scale corpus can often be applied to downstream natural language processing tasks. This section will demonstrate how to use these pre-trained word vectors to find synonyms and analogies. We will continue to apply pre-trained word vectors in subsequent sections.

### 15.7.1 Using Pre-trained Word Vectors

MXNet's `contrib.text` package provides functions and classes related to natural language processing (see the [GluonNLP<sup>201</sup>](#) tool package for more details). Next, let us check out names of the provided pre-trained word embeddings.

```
from mxnet import nd
from mxnet.contrib import text

text.embedding.get_pretrained_file_names().keys()

dict_keys(['glove', 'fasttext'])
```

<sup>200</sup> <https://discuss.mxnet.io/t/2389>

<sup>201</sup> <https://gluon-nlp.mxnet.io/>

Given the name of the word embedding, we can see which pre-trained models are provided by the word embedding. The word vector dimensions of each model may be different or obtained by pre-training on different data sets.

```
print(text.embedding.get_pretrained_file_names('glove'))
```

```
['glove.42B.300d.txt', 'glove.6B.50d.txt', 'glove.6B.100d.txt', 'glove.6B.200d.txt',
 ↪'glove.6B.300d.txt', 'glove.840B.300d.txt', 'glove.twitter.27B.25d.txt', 'glove.
 ↪twitter.27B.50d.txt', 'glove.twitter.27B.100d.txt', 'glove.twitter.27B.200d.txt']
```

The general naming conventions for pre-trained GloVe models are “model.(data set.)number of words in data set.word vector dimension.txt”. For more information, please refer to the GloVe and fastText project sites [2,3]. Below, we use a 50-dimensional GloVe word vector based on Wikipedia subset pre-training. The corresponding word vector is automatically downloaded the first time we create a pre-trained word vector instance.

```
glove_6b50d = text.embedding.create(
    'glove', pretrained_file_name='glove.6B.50d.txt')
```

Print the dictionary size. The dictionary contains 400,000 words and a special unknown token.

```
len(glove_6b50d)
```

```
400001
```

We can use a word to get its index in the dictionary, or we can get the word from its index.

```
glove_6b50d.token_to_idx['beautiful'], glove_6b50d.idx_to_token[3367]
```

```
(3367, 'beautiful')
```

## 15.7.2 Applying Pre-trained Word Vectors

Below, we demonstrate the application of pre-trained word vectors, using GloVe as an example.

### Finding Synonyms

Here, we re-implement the algorithm used to search for synonyms by cosine similarity introduced in Section 15.1

In order to reuse the logic for seeking the  $k$  nearest neighbors when seeking analogies, we encapsulate this part of the logic separately in the `knn` ( $k$ -nearest neighbors) function.

```
def knn(W, x, k):
    # The added 1e-9 is for numerical stability
    cos = nd.dot(W, x.reshape((-1,))) / (
        (nd.sum(W * W, axis=1) + 1e-9).sqrt() * nd.sum(x * x).sqrt())
    topk = nd.topk(cos, k=k, ret_type='indices').asnumpy().astype('int32')
    return topk, [cos[i].asscalar() for i in topk]
```

Then, we search for synonyms by pre-training the word vector instance `embed`.

```
def get_similar_tokens(query_token, k, embed):
    topk, cos = knn(embed.idx_to_vec,
                    embed.get_vecs_by_tokens([query_token]), k+1)
    for i, c in zip(topk[1:], cos[1:]): # Remove input words
        print('cosine sim=% .3f: %s' % (c, (embed.idx_to_token[i])))
```

The dictionary of pre-trained word vector instance `glove_6b50d` already created contains 400,000 words and a special unknown token. Excluding input words and unknown words, we search for the three words that are the most similar in meaning to “chip”.

```
get_similar_tokens('chip', 3, glove_6b50d)
```

```
cosine sim=0.856: chips
cosine sim=0.749: intel
cosine sim=0.749: electronics
```

Next, we search for the synonyms of “baby” and “beautiful”.

```
get_similar_tokens('baby', 3, glove_6b50d)
```

```
cosine sim=0.839: babies
cosine sim=0.800: boy
cosine sim=0.792: girl
```

```
get_similar_tokens('beautiful', 3, glove_6b50d)
```

```
cosine sim=0.921: lovely
cosine sim=0.893: gorgeous
cosine sim=0.830: wonderful
```

## Finding Analogies

In addition to seeking synonyms, we can also use the pre-trained word vector to seek the analogies between words. For example, “man”:“woman”::“son”:“daughter” is an example of analogy, “man” is to “woman” as “son” is to “daughter”. The problem of seeking analogies can be defined as follows: for four words in the analogical relationship  $a : b :: c : d$ , given the first three words,  $a$ ,  $b$  and  $c$ , we want to find  $d$ . Assume the word vector for the word  $w$  is  $\text{vec}(w)$ . To solve the analogy problem, we need to find the word vector that is most similar to the result vector of  $\text{vec}(c) + \text{vec}(b) - \text{vec}(a)$ .

```
def get_analogy(token_a, token_b, token_c, embed):
    vecs = embed.get_vecs_by_tokens([token_a, token_b, token_c])
    x = vecs[1] - vecs[0] + vecs[2]
    topk, cos = knn(embed.idx_to_vec, x, 1)
    return embed.idx_to_token[topk[0]] # Remove unknown words
```

Verify the “male-female” analogy.

```
get_analogy('man', 'woman', 'son', glove_6b50d)
```

```
'daughter'
```

“Capital-country” analogy: “beijing” is to “china” as “tokyo” is to what? The answer should be “japan”.

```
get_analogy('beijing', 'china', 'tokyo', glove_6b50d)
```

```
'japan'
```

“Adjective-superlative adjective” analogy: “bad” is to “worst” as “big” is to what? The answer should be “biggest”.

```
get_analogy('bad', 'worst', 'big', glove_6b50d)
```

```
'biggest'
```

“Present tense verb-past tense verb” analogy: “do” is to “did” as “go” is to what? The answer should be “went”.

```
get_analogy('do', 'did', 'go', glove_6b50d)
```

```
'went'
```

### 15.7.3 Summary

- Word vectors pre-trained on a large-scale corpus can often be applied to downstream natural language processing tasks.
- We can use pre-trained word vectors to seek synonyms and analogies.

### 15.7.4 Exercises

- Test the fastText results.
- If the dictionary is extremely large, how can we accelerate finding synonyms and analogies?

### 15.7.5 Scan the QR Code to Discuss<sup>202</sup>



## 15.8 Text Classification and Data Sets

Text classification is a common task in natural language processing, which transforms a sequence of text of indefinite length into a category of text. It’s similar to the image classification, the most frequently used application in this book, e.g. Section 4.5. The only difference is that, rather than an image, text classification’s example is a text sentence.

<sup>202</sup> <https://discuss.mxnet.io/t/2390>

This section will focus on loading data for one of the sub-questions in this field: using text sentiment classification to analyze the emotions of the text's author. This problem is also called sentiment analysis and has a wide range of applications. For example, we can analyze user reviews of products to obtain user satisfaction statistics, or analyze user sentiments about market conditions and use it to predict future trends.

```
import d2l
from mxnet import gluon, nd
import os
import tarfile
```

### 15.8.1 Text Sentiment Classification Data

We use Stanford's Large Movie Review Dataset as the data set for text sentiment classification[1]. This data set is divided into two data sets for training and testing purposes, each containing 25,000 movie reviews downloaded from IMDb. In each data set, the number of comments labeled as “positive” and “negative” is equal.

#### Reading Data

We first download this data set to the “`../data`” path and extract it to “`../data/aclImdb`”.

```
# Save to the d2l package.
def download_imdb(data_dir='../data'):
    url = 'http://ai.stanford.edu/~amaas/data/sentiment/aclImdb_v1.tar.gz'
    fname = gluon.utils.download(url, data_dir)
    with tarfile.open(fname, 'r') as f:
        f.extractall(data_dir)

download_imdb()
```

Next, read the training and test data sets. Each example is a review and its corresponding label: 1 indicates “positive” and 0 indicates “negative”.

```
# Save to the d2l package.
def read_imdb(folder='train', data_dir='../data'):
    data, labels = [], []
    for label in ['pos', 'neg']:
        folder_name = os.path.join(data_dir, 'aclImdb', folder, label)
        for file in os.listdir(folder_name):
            with open(os.path.join(folder_name, file), 'rb') as f:
                review = f.read().decode('utf-8').replace('\n', '')
            data.append(review)
            labels.append(1 if label == 'pos' else 0)
    return data, labels

train_data = read_imdb('train')
print('# trainings:', len(train_data[0]))
for x, y in zip(train_data[0][:3], train_data[1][:3]):
    print('label:', y, 'review:', x[0:60])
```

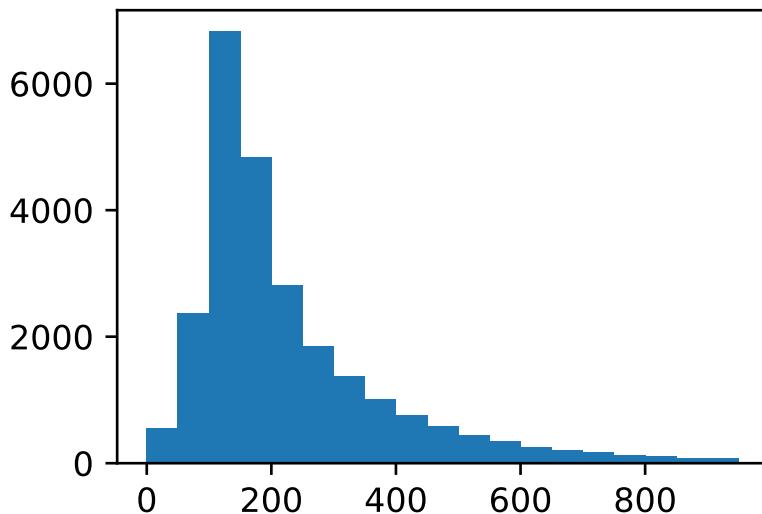
```
# trainings: 25000
label: 1 review: Normally the best way to annoy me in a film is to include so
label: 1 review: The Bible teaches us that the love of money is the root of a
label: 1 review: Being someone who lists Night of the Living Dead at number t
```

## Tokenization and Vocabulary

We use a word as a token, and then create a dictionary based on the training data set.

```
train_tokens = d2l.tokenize(train_data[0], token='word')
vocab = d2l.Vocab(train_tokens, min_freq=5)

d2l.set_figsize((3.5, 2.5))
d2l.plt.hist([len(line) for line in train_tokens], bins=range(0,1000,50));
```



## Padding to the Same Length

Because the reviews have different lengths, so they cannot be directly combined into mini-batches. Here we fix the length of each comment to 500 by truncating or adding “<unk>” indices.

```
num_steps = 500 # sequence length
train_features = nd.array([d2l.trim_pad(vocab[line], num_steps, vocab.unk)
                           for line in train_tokens])
train_features.shape
```

```
(25000, 500)
```

## Create Data Iterator

Now, we will create a data iterator. Each iteration will return a mini-batch of data.

```
train_iter = d2l.load_array((train_features, train_data[1]), 64)

for X, y in train_iter:
    print('X', X.shape, 'y', y.shape)
    break
'# batches:', len(train_iter)
```

```
X (64, 500) y (64,)
```

```
('# batches:', 391)
```

### 15.8.2 Put All Things Together

Lastly, we will save a function `load_data_imdb` into `d2l`, which returns the vocabulary and data iterators.

```
# Save to the d2l package.
def load_data_imdb(batch_size, num_steps=500):
    download_imdb()
    train_data, test_data = read_imdb('train'), read_imdb('test')
    train_tokens = d2l.tokenize(train_data[0], token='word')
    test_tokens = d2l.tokenize(test_data[0], token='word')
    vocab = d2l.Vocab(train_tokens, min_freq=5)
    train_features = nd.array([d2l.trim_pad(vocab[line], num_steps, vocab.unk)
                               for line in train_tokens])
    test_features = nd.array([d2l.trim_pad(vocab[line], num_steps, vocab.unk)
                             for line in test_tokens])
    train_iter = d2l.load_array((train_features, train_data[1]), batch_size)
    test_iter = d2l.load_array((test_features, test_data[1]), batch_size,
                               is_train=False)
    return train_iter, test_iter, vocab
```

### 15.8.3 Summary

## 15.9 Text Sentiment Classification: Using Recurrent Neural Networks

Similar to search synonyms and analogies, text classification is also a downstream application of word embedding. In this section, we will apply pre-trained word vectors and bidirectional recurrent neural networks with multiple hidden layers [44]. We will use them to determine whether a text sequence of indefinite length contains positive or negative emotion. Import the required package or module before starting the experiment.

```
import d2l
from mxnet import gluon, init, nd
from mxnet.gluon import nn, rnn
from mxnet.contrib import text

batch_size = 64
train_iter, test_iter, vocab = d2l.load_data_imdb(batch_size)
```

### 15.9.1 Use a Recurrent Neural Network Model

In this model, each word first obtains a feature vector from the embedding layer. Then, we further encode the feature sequence using a bidirectional recurrent neural network to obtain sequence information. Finally, we transform the encoded sequence information to output through the fully connected layer. Specifically, we can concatenate hidden states of bidirectional long-short term memory in the initial time step and final time step and pass it to the output layer classification as encoded feature sequence information. In the `BiRNN` class implemented below, the `Embedding` instance is the embedding layer, the `LSTM` instance is the hidden layer for sequence encoding, and the `Dense` instance is the output layer for generated classification results.

```
class BiRNN(nn.Block):
    def __init__(self, vocab_size, embed_size, num_hiddens, num_layers, **kwargs):
        super(BiRNN, self).__init__(**kwargs)
        self.embedding = nn.Embedding(vocab_size, embed_size)
        # Set Bidirectional to True to get a bidirectional recurrent neural
        # network
        self.encoder = rnn.LSTM(num_hiddens, num_layers=num_layers,
                               bidirectional=True, input_size=embed_size)
        self.decoder = nn.Dense(2)

    def forward(self, inputs):
        # The shape of inputs is (batch size, number of words). Because LSTM
        # needs to use sequence as the first dimension, the input is
        # transformed and the word feature is then extracted. The output shape
        # is (number of words, batch size, word vector dimension).
        embeddings = self.embedding(inputs.T)
        # Since the input (embeddings) is the only argument passed into
        # rnn.LSTM, it only returns the hidden states of the last hidden layer
        # at different time step (outputs). The shape of outputs is
        # (number of words, batch size, 2 * number of hidden units).
        outputs = self.encoder(embeddings)
        # Concatenate the hidden states of the initial time step and final
        # time step to use as the input of the fully connected layer. Its
        # shape is (batch size, 4 * number of hidden units)
        encoding = nd.concat(outputs[0], outputs[-1])
        outs = self.decoder(encoding)
        return outs
```

Create a bidirectional recurrent neural network with two hidden layers.

```
embed_size, num_hiddens, num_layers, ctx = 100, 100, 2, d2l.try_all_gpus()
net = BiRNN(len(vocab), embed_size, num_hiddens, num_layers)
net.initialize(init.Xavier(), ctx=ctx)
```

#### Load Pre-trained Word Vectors

Because the training data set for sentiment classification is not very large, in order to deal with overfitting, we will directly use word vectors pre-trained on a larger corpus as the feature vectors of all words. Here, we load a 100-dimensional GloVe word vector for each word in the dictionary `vocab`.

```
glove_embedding = text.embedding.create(
    'glove', pretrained_file_name='glove.6B.100d.txt')
```

Query the word vectors that in our vocabulary.

```
embeds = glove_embedding.get_vecs_by_tokens(vocab.idx_to_token)
embeds.shape
```

```
(49339, 100)
```

Then, we will use these word vectors as feature vectors for each word in the reviews. Note that the dimensions of the pre-trained word vectors need to be consistent with the embedding layer output size `embed_size` in the created model. In addition, we no longer update these word vectors during training.

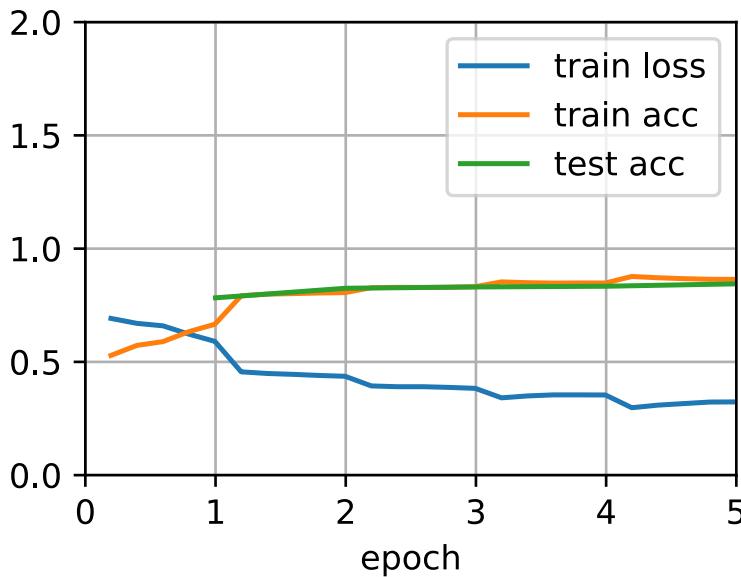
```
net.embedding.weight.set_data(embeds)
net.embedding.collect_params().setattr('grad_req', 'null')
```

## Train and Evaluate the Model

Now, we can start training.

```
lr, num_epochs = 0.01, 5
trainer = gluon.Trainer(net.collect_params(), 'adam', {'learning_rate': lr})
loss = gluon.loss.SoftmaxCrossEntropyLoss()
d2l.train_ch12(net, train_iter, test_iter, loss, trainer, num_epochs, ctx)
```

```
loss 0.323, train acc 0.864, test acc 0.845
887.7 examples/sec on [gpu(0), gpu(1)]
```



Finally, define the prediction function.

```
# Save to the d2l package.
def predict_sentiment(net, vocab, sentence):
    sentence = nd.array(vocab[sentence.split()], ctx=d2l.try_gpu())
    label = nd.argmax(net(sentence.reshape((1, -1))), axis=1)
    return 'positive' if label.asscalar() == 1 else 'negative'
```

Then, use the trained model to classify the sentiments of two simple sentences.

```
predict_sentiment(net, vocab, 'this movie is so great')
```

```
'positive'
```

```
predict_sentiment(net, vocab, 'this movie is so bad')
```

```
'negative'
```

### 15.9.2 Summary

- Text classification transforms a sequence of text of indefinite length into a category of text. This is a downstream application of word embedding.
- We can apply pre-trained word vectors and recurrent neural networks to classify the emotions in a text.

### 15.9.3 Exercises

- Increase the number of epochs. What accuracy rate can you achieve on the training and testing data sets? What about trying to re-tune other hyper-parameters?
- Will using larger pre-trained word vectors, such as 300-dimensional GloVe word vectors, improve classification accuracy?
- Can we improve the classification accuracy by using the spaCy word tokenization tool? You need to install spaCy: `pip install spacy` and install the English package: `python -m spacy download en`. In the code, first import spacy: `import spacy`. Then, load the spacy English package: `spacy_en = spacy.load('en')`. Finally, define the function `def tokenizer(text): return [tok.text for tok in spacy_en.tokenizer(text)]` and replace the original `tokenizer` function. It should be noted that GloVe's word vector uses “\_” to connect each word when storing noun phrases. For example, the phrase “new york” is represented as “new-york” in GloVe. After using spaCy tokenization, “new york” may be stored as “new york”.

### 15.9.4 Scan the QR Code to Discuss<sup>203</sup>



<sup>203</sup> <https://discuss.mxnet.io/t/2391>

## 15.10 Text Sentiment Classification: Using Convolutional Neural Networks (textCNN)

In Section 8, we explored how to process two-dimensional image data with two-dimensional convolutional neural networks. In the previous language models and text classification tasks, we treated text data as a time series with only one dimension, and naturally, we used recurrent neural networks to process such data. In fact, we can also treat text as a one-dimensional image, so that we can use one-dimensional convolutional neural networks to capture associations between adjacent words. This section describes a groundbreaking approach to applying convolutional neural networks to text analysis: textCNN [30]. First, import the packages and modules required for the experiment.

```
import d2l
from mxnet import gluon, init, nd
from mxnet.contrib import text
from mxnet.gluon import nn

batch_size = 64
train_iter, test_iter, vocab = d2l.load_data_imdb(batch_size)
```

### 15.10.1 One-dimensional Convolutional Layer

Before introducing the model, let us explain how a one-dimensional convolutional layer works. Like a two-dimensional convolutional layer, a one-dimensional convolutional layer uses a one-dimensional cross-correlation operation. In the one-dimensional cross-correlation operation, the convolution window starts from the leftmost side of the input array and slides on the input array from left to right successively. When the convolution window slides to a certain position, the input subarray in the window and kernel array are multiplied and summed by element to get the element at the corresponding location in the output array. As shown in Figure 12.4, the input is a one-dimensional array with a width of 7 and the width of the kernel array is 2. As we can see, the output width is  $7 - 2 + 1 = 6$  and the first element is obtained by performing multiplication by element on the leftmost input subarray with a width of 2 and kernel array and then summing the results.

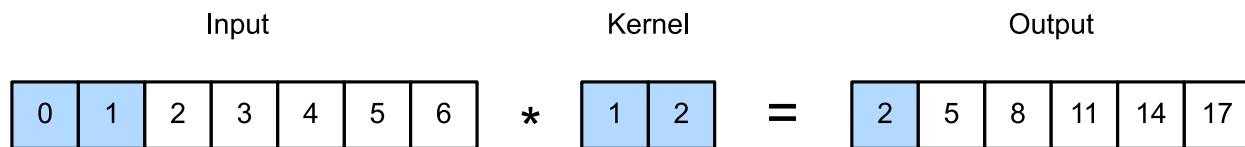


Fig. 15.10.1: One-dimensional cross-correlation operation. The shaded parts are the first output element as well as the input and kernel array elements used in its calculation:  $0 \times 1 + 1 \times 2 = 2$ .

Next, we implement one-dimensional cross-correlation in the `corr1d` function. It accepts the input array `X` and kernel array `K` and outputs the array `Y`.

```
def corr1d(X, K):
    w = K.shape[0]
    Y = nd.zeros((X.shape[0] - w + 1))
    for i in range(Y.shape[0]):
        Y[i] = (X[i:i+w] * K).sum()
    return Y
```

Now, we will reproduce the results of the one-dimensional cross-correlation operation in Figure 12.4.

```
X, K = nd.array([0, 1, 2, 3, 4, 5, 6]), nd.array([1, 2])
corr1d(X, K)
```

```
[ 2.  5.  8. 11. 14. 17.]
<NDArray 6 @cpu(0)>
```

The one-dimensional cross-correlation operation for multiple input channels is also similar to the two-dimensional cross-correlation operation for multiple input channels. On each channel, it performs the one-dimensional cross-correlation operation on the kernel and its corresponding input and adds the results of the channels to get the output. Figure 12.5 shows a one-dimensional cross-correlation operation with three input channels.

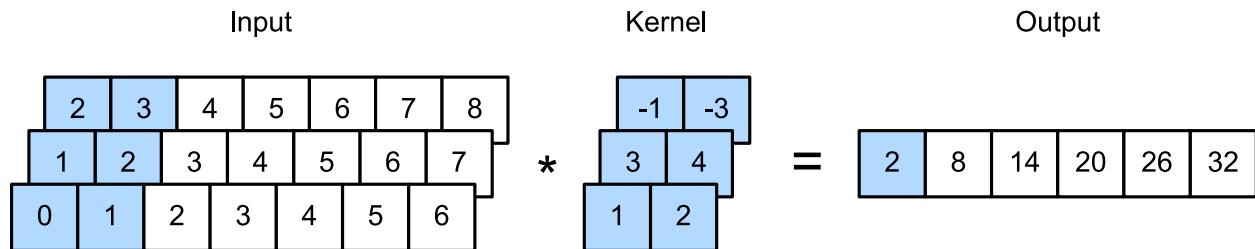


Fig. 15.10.2: One-dimensional cross-correlation operation with three input channels. The shaded parts are the first output element as well as the input and kernel array elements used in its calculation:  $0 \times 1 + 1 \times 2 + 1 \times 3 + 2 \times 4 + 2 \times (-1) + 3 \times (-3) = 2$ .

Now, we reproduce the results of the one-dimensional cross-correlation operation with multi-input channel in Figure 12.5.

```
def corr1d_multi_in(X, K):
    # First, we traverse along the 0th dimension (channel dimension) of X and
    # K. Then, we add them together by using * to turn the result list into a
    # positional argument of the add_n function
    return nd.add_n(*[corr1d(x, k) for x, k in zip(X, K)])

X = nd.array([[0, 1, 2, 3, 4, 5, 6],
              [1, 2, 3, 4, 5, 6, 7],
              [2, 3, 4, 5, 6, 7, 8]])
K = nd.array([[1, 2], [3, 4], [-1, -3]])
corr1d_multi_in(X, K)
```

```
[ 2.  8. 14. 20. 26. 32.]
<NDArray 6 @cpu(0)>
```

The definition of a two-dimensional cross-correlation operation tells us that a one-dimensional cross-correlation operation with multiple input channels can be regarded as a two-dimensional cross-correlation operation with a single input channel. As shown in Figure 12.6, we can also present the one-dimensional cross-correlation operation with multiple input channels in Figure 12.5 as the equivalent two-dimensional cross-correlation operation with a single input channel. Here, the height of the kernel is equal to the height of the input.

Both the outputs in Figure 12.4 and Figure 12.5 have only one channel. We discussed how to specify multiple output channels in a two-dimensional convolutional layer in Section 8.4. Similarly, we can also

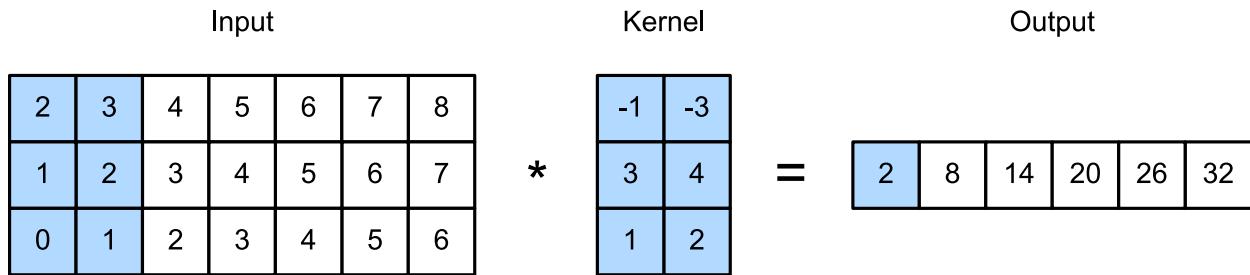


Fig. 15.10.3: Two-dimensional cross-correlation operation with a single input channel. The highlighted parts are the first output element and the input and kernel array elements used in its calculation:  $2 \times (-1) + 3 \times (-3) + 1 \times 3 + 2 \times 4 + 0 \times 1 + 1 \times 2 = 2$ .

specify multiple output channels in the one-dimensional convolutional layer to extend the model parameters in the convolutional layer.

### 15.10.2 Max-Over-Time Pooling Layer

Similarly, we have a one-dimensional pooling layer. The max-over-time pooling layer used in TextCNN actually corresponds to a one-dimensional global maximum pooling layer. Assuming that the input contains multiple channels, and each channel consists of values on different time steps, the output of each channel will be the largest value of all time steps in the channel. Therefore, the input of the max-over-time pooling layer can have different time steps on each channel.

To improve computing performance, we often combine timing examples of different lengths into a mini-batch and make the lengths of each timing example in the batch consistent by appending special characters (such as 0) to the end of shorter examples. Naturally, the added special characters have no intrinsic meaning. Because the main purpose of the max-over-time pooling layer is to capture the most important features of timing, it usually allows the model to be unaffected by the manually added characters.

### 15.10.3 The TextCNN Model

TextCNN mainly uses a one-dimensional convolutional layer and max-over-time pooling layer. Suppose the input text sequence consists of  $n$  words, and each word is represented by a  $d$ -dimension word vector. Then the input example has a width of  $n$ , a height of 1, and  $d$  input channels. The calculation of textCNN can be mainly divided into the following steps:

1. Define multiple one-dimensional convolution kernels and use them to perform convolution calculations on the inputs. Convolution kernels with different widths may capture the correlation of different numbers of adjacent words.
2. Perform max-over-time pooling on all output channels, and then concatenate the pooling output values of these channels in a vector.
3. The concatenated vector is transformed into the output for each category through the fully connected layer. A dropout layer can be used in this step to deal with overfitting.

Figure 12.7 gives an example to illustrate the textCNN. The input here is a sentence with 11 words, with each word represented by a 6-dimensional word vector. Therefore, the input sequence has a width of 11 and 6 input channels. We assume there are two one-dimensional convolution kernels with widths of 2 and 4, and 4 and 5 output channels, respectively. Therefore, after one-dimensional convolution calculation, the width of the four output channels is  $11 - 2 + 1 = 10$ , while the width of the other five channels is  $11 - 4 + 1 = 8$ . Even though the width of each channel is different, we can still perform max-over-time pooling for each channel

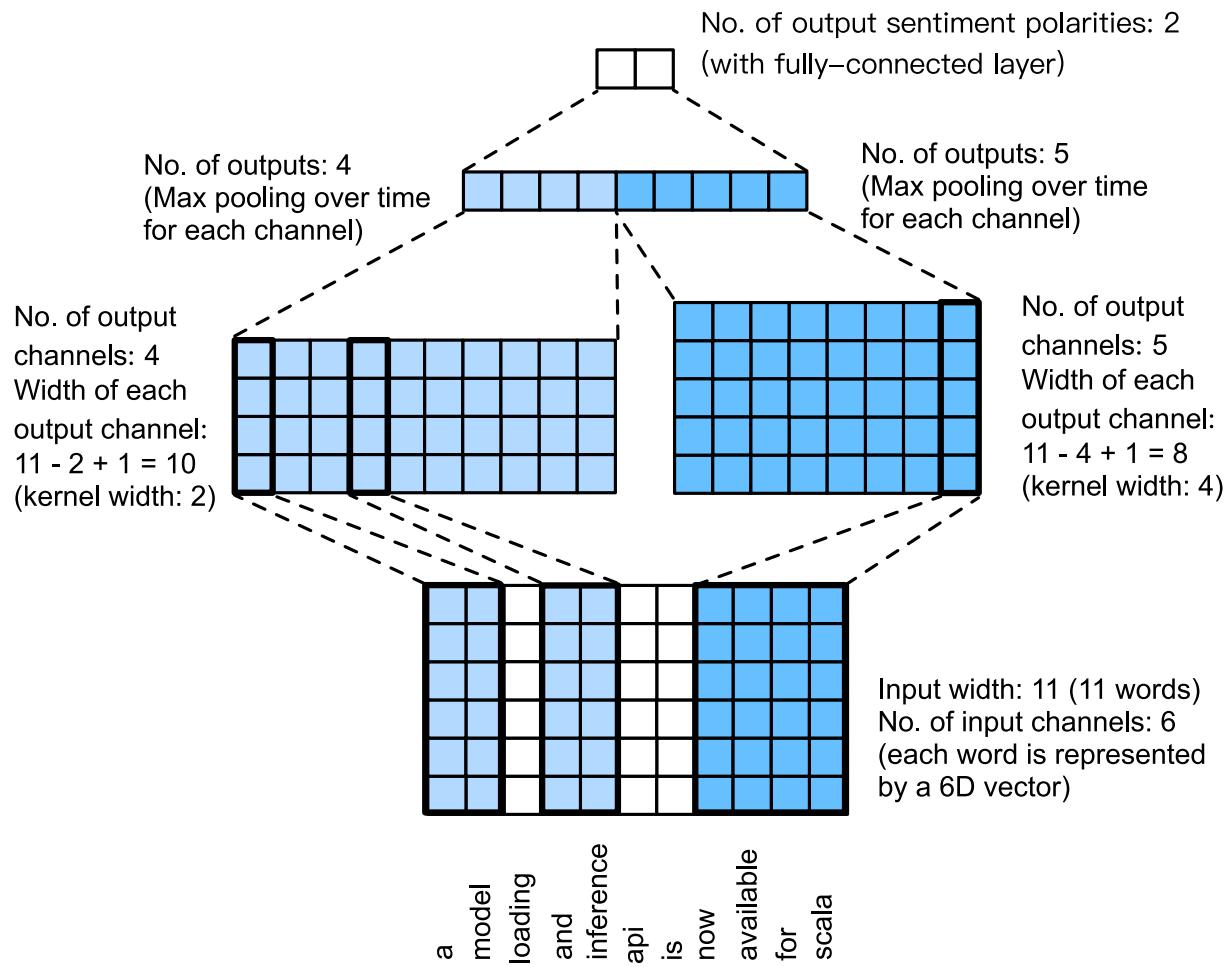


Fig. 15.10.4: TextCNN design.

and concatenate the pooling outputs of the 9 channels into a 9-dimensional vector. Finally, we use a fully connected layer to transform the 9-dimensional vector into a 2-dimensional output: positive sentiment and negative sentiment predictions.

Next, we will implement a textCNN model. Compared with the previous section, in addition to replacing the recurrent neural network with a one-dimensional convolutional layer, here we use two embedding layers, one with a fixed weight and another that participates in training.

```
class TextCNN(nn.Block):
    def __init__(self, vocab_size, embed_size, kernel_sizes, num_channels,
                 **kwargs):
        super(TextCNN, self).__init__(**kwargs)
        self.embedding = nn.Embedding(vocab_size, embed_size)
        # The embedding layer does not participate in training
        self.constant_embedding = nn.Embedding(vocab_size, embed_size)
        self.dropout = nn.Dropout(0.5)
        self.decoder = nn.Dense(2)
        # The max-over-time pooling layer has no weight, so it can share an
        # instance
        self.pool = nn.GlobalMaxPool1D()
        # Create multiple one-dimensional convolutional layers
        self.convs = nn.Sequential()
        for c, k in zip(num_channels, kernel_sizes):
            self.convs.add(nn.Conv1D(c, k, activation='relu'))

    def forward(self, inputs):
        # Concatenate the output of two embedding layers with shape of
        # (batch size, number of words, word vector dimension) by word vector
        embeddings = nd.concat(
            self.embedding(inputs), self.constant_embedding(inputs), dim=2)
        # According to the input format required by Conv1D, the word vector
        # dimension, that is, the channel dimension of the one-dimensional
        # convolutional layer, is transformed into the previous dimension
        embeddings = embeddings.transpose((0, 2, 1))
        # For each one-dimensional convolutional layer, after max-over-time
        # pooling, an NDArray with the shape of (batch size, channel size, 1)
        # can be obtained. Use the flatten function to remove the last
        # dimension and then concatenate on the channel dimension
        encoding = nd.concat(*[nd.flatten(
            self.pool(conv(embeddings))) for conv in self.convs], dim=1)
        # After applying the dropout method, use a fully connected layer to
        # obtain the output
        outputs = self.decoder(self.dropout(encoding))
        return outputs
```

Create a TextCNN instance. It has 3 convolutional layers with kernel widths of 3, 4, and 5, all with 100 output channels.

```
embed_size, kernel_sizes, nums_channels = 100, [3, 4, 5], [100, 100, 100]
ctx = d2l.try_all_gpus()
net = TextCNN(len(vocab), embed_size, kernel_sizes, nums_channels)
net.initialize(init.Xavier(), ctx=ctx)
```

## Load Pre-trained Word Vectors

As in the previous section, load pre-trained 100-dimensional GloVe word vectors and initialize the embedding layers `embedding` and `constant_embedding`. Here, the former participates in training while the latter has a fixed weight.

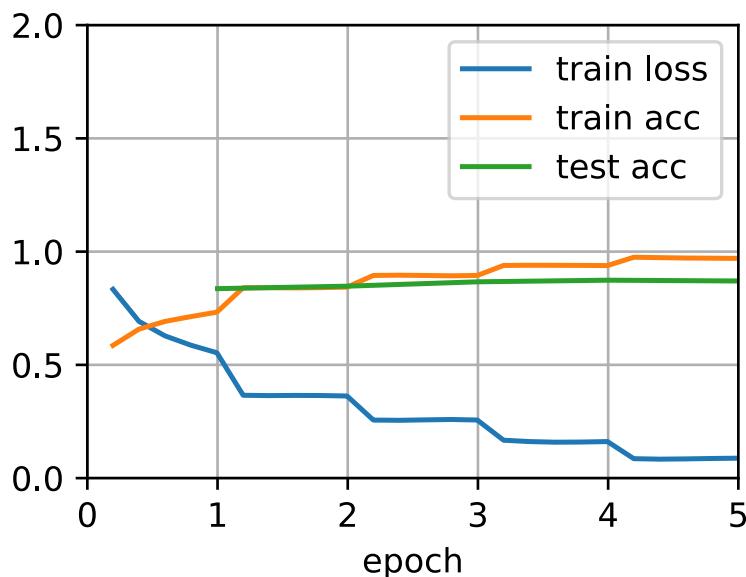
```
glove_embedding = text.embedding.create(
    'glove', pretrained_file_name='glove.6B.100d.txt')
embeds = glove_embedding.get_vecs_by_tokens(vocab.idx_to_token)
net.embedding.weight.set_data(embeds)
net.constant_embedding.weight.set_data(embeds)
net.constant_embedding.collect_params().setattr('grad_req', 'null')
```

## Train and Evaluate the Model

Now we can train the model.

```
lr, num_epochs = 0.001, 5
trainer = gluon.Trainer(net.collect_params(), 'adam', {'learning_rate': lr})
loss = gluon.loss.SoftmaxCrossEntropyLoss()
d2l.train_ch12(net, train_iter, test_iter, loss, trainer, num_epochs, ctx)
```

```
loss 0.088, train acc 0.970, test acc 0.870
3090.2 examples/sec on [gpu(0), gpu(1)]
```



Below, we use the trained model to classify sentiments of two simple sentences.

```
d2l.predict_sentiment(net, vocab, 'this movie is so great')
```

```
'positive'
```

```
d2l.predict_sentiment(net, vocab, 'this movie is so bad')
```

```
'negative'
```

#### 15.10.4 Summary

- We can use one-dimensional convolution to process and analyze timing data.
- A one-dimensional cross-correlation operation with multiple input channels can be regarded as a two-dimensional cross-correlation operation with a single input channel.
- The input of the max-over-time pooling layer can have different numbers of time steps on each channel.
- TextCNN mainly uses a one-dimensional convolutional layer and max-over-time pooling layer.

#### 15.10.5 Exercises

- Tune the hyper-parameters and compare the two sentiment analysis methods, using recurrent neural networks and using convolutional neural networks, as regards accuracy and operational efficiency.
- Can you further improve the accuracy of the model on the test set by using the three methods introduced in the previous section: tuning hyper-parameters, using larger pre-trained word vectors, and using the spaCy word tokenization tool?
- What other natural language processing tasks can you use textCNN for?

#### 15.10.6 Scan the QR Code to Discuss<sup>204</sup>



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<sup>204</sup> <https://discuss.mxnet.io/t/2392>

## GENERATIVE ADVERSARIAL NETWORKS

### 16.1 Generative Adversarial Networks

Throughout most of this book, we've talked about how to make predictions. In some form or another, we used deep neural networks learned mappings from data points to labels. This kind of learning is called discriminative learning, as in, we'd like to be able to discriminate between photos of cats and photos of dogs. Classifiers and regressors are both examples of discriminative learning. And neural networks trained by backpropagation have upended everything we thought we knew about discriminative learning on large complicated datasets. Classification accuracies on high-res images has gone from useless to human-level (with some caveats) in just 5-6 years. We'll spare you another spiel about all the other discriminative tasks where deep neural networks do astoundingly well.

But there's more to machine learning than just solving discriminative tasks. For example, given a large dataset, without any labels, we might want to learn a model that concisely captures the characteristics of this data. Given such a model, we could sample synthetic data points that resemble the distribution of the training data. For example, given a large corpus of photographs of faces, we might want to be able to generate a new photorealistic image that looks like it might plausibly have come from the same dataset. This kind of learning is called generative modeling.

Until recently, we had no method that could synthesize novel photorealistic images. But the success of deep neural networks for discriminative learning opened up new possibilities. One big trend over the last three years has been the application of discriminative deep nets to overcome challenges in problems that we don't generally think of as supervised learning problems. The recurrent neural network language models are one example of using a discriminative network (trained to predict the next character) that once trained can act as a generative model.

In 2014, a breakthrough paper introduced Generative adversarial networks (GANs) [20], a clever new way to leverage the power of discriminative models to get good generative models. At their heart, GANs rely on the idea that a data generator is good if we cannot tell fake data apart from real data. In statistics, this is called a two-sample test - a test to answer the question whether datasets  $X = \{x_1, \dots, x_n\}$  and  $X' = \{x'_1, \dots, x'_n\}$  were drawn from the same distribution. The main difference between most statistics papers and GANs is that the latter use this idea in a constructive way. In other words, rather than just training a model to say "hey, these two datasets don't look like they came from the same distribution", they use the [two-sample test<sup>205</sup>](#) to provide training signal to a generative model. This allows us to improve the data generator until it generates something that resembles the real data. At the very least, it needs to fool the classifier. And if our classifier is a state of the art deep neural network.

The GANs architecture is illustrated in Fig. 16.1.1. As you can see, there are two pieces to GANs - first off, we need a device (say, a deep network but it really could be anything, such as a game rendering engine) that might potentially be able to generate data that looks just like the real thing. If we are dealing with images, this needs to generate images. If we're dealing with speech, it needs to generate audio sequences, and so on. We call this the generator network. The second component is the discriminator network. It attempts

<sup>205</sup> [https://en.wikipedia.org/wiki/Two-sample\\_hypothesis\\_testing](https://en.wikipedia.org/wiki/Two-sample_hypothesis_testing)

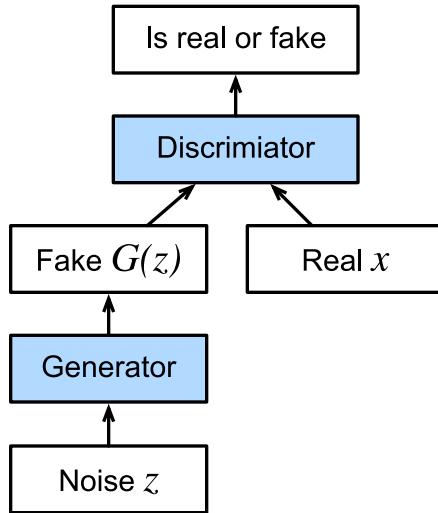


Fig. 16.1.1: Generative Adversarial Networks

to distinguish fake and real data from each other. Both networks are in competition with each other. The generator network attempts to fool the discriminator network. At that point, the discriminator network adapts to the new fake data. This information, in turn is used to improve the generator network, and so on.

The discriminator is a binary classifier to distinguish if the input  $x$  is real (from real data) or fake (from the generator). Typically, the discriminator outputs a scalar prediction  $o \in \mathbb{R}$  for input  $\mathbf{x}$ , such as using a dense layer with hidden size 1, and then applies sigmoid function to obtain the predicted probability  $D(\mathbf{x}) = 1/(1 + e^{-o})$ . Assume the label  $y$  for true data is 1 and 0 for fake data. We train the discriminator to minimize the cross-entropy loss, i.e.

$$\min -y \log D(\mathbf{x}) - (1 - y) \log(1 - D(\mathbf{x})), \quad (16.1.1)$$

For the generator, it first draws some parameter  $\mathbf{z} \in \mathbb{R}^d$  from a source of randomness, e.g. a normal distribution  $\mathbf{z} \sim (0, 1)$ . We often call  $\mathbf{z}$  the latent variable. It then applies a function to generate  $\mathbf{x}' = G(\mathbf{z})$ . The goal of the generator is to fool the discriminator to classify  $\mathbf{x}'$  as true data. In other words, we update the parameters of the generator to maximize the cross-entropy loss when  $y = 0$ , i.e.

$$\max -\log(1 - D(\mathbf{x}')). \quad (16.1.2)$$

If the discriminator does a perfect job, then  $D(\mathbf{x}') \approx 1$  so the above loss near 0, which results the gradients are too small to make a good progress for the discriminator. So commonly we minimize the following loss

$$\max \log(D(\mathbf{x}')), \quad (16.1.3)$$

which is just feed  $\mathbf{x}'$  into the discriminator but giving label  $y = 1$ .

Many of the GANs applications are in the context of images. As a demonstration purpose, we're going to content ourselves with fitting a much simpler distribution first. We will illustrate what happens if we use GANs to build the world's most inefficient estimator of parameters for a Gaussian. Let's get started.

```
%matplotlib inline
import d2l
from mxnet import nd, gluon, autograd, init
from mxnet.gluon import nn
```

### 16.1.1 Generate some “real” data

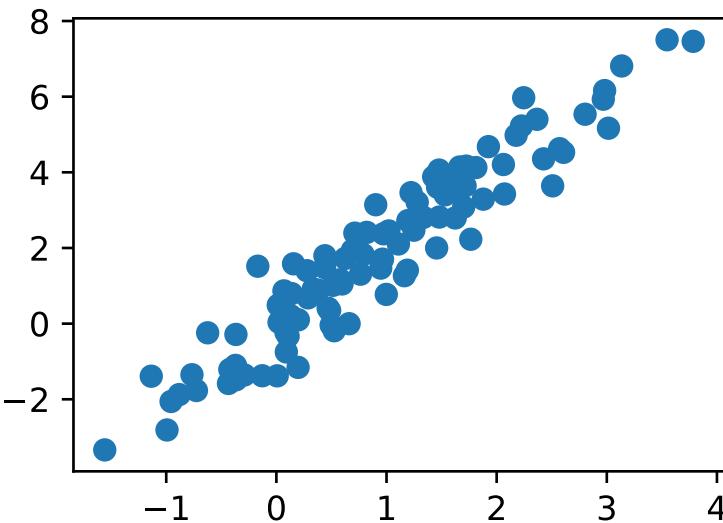
Since this is going to be the world’s lamest example, we simply generate data drawn from a Gaussian.

```
X = nd.random.normal(shape=(1000, 2))
A = nd.array([[1, 2], [-0.1, 0.5]])
b = nd.array([1, 2])
data = nd.dot(X, A) + b
```

Let’s see what we got. This should be a Gaussian shifted in some rather arbitrary way with mean  $b$  and covariance matrix  $A^T A$ .

```
d2l.set_figsize((3.5, 2.5))
#d2l.plt.figure(figsize=())
d2l.plt.scatter(data[:100,0].asnumpy(), data[:100,1].asnumpy());
print("The covariance matrix is", nd.dot(A.T,A))
```

```
The covariance matrix is
[[1.01 1.95]
 [1.95 4.25]]
<NDArray 2x2 @cpu(0)>
```



```
batch_size = 8
data_iter = d2l.load_array((data,), batch_size)
```

### 16.1.2 Generator

Our generator network will be the simplest network possible - a single layer linear model. This is since we’ll be driving that linear network with a Gaussian data generator. Hence, it literally only needs to learn the parameters to fake things perfectly.

```
net_G = nn.Sequential()
net_G.add(nn.Dense(2))
```

### 16.1.3 Discriminator

For the discriminator we will be a bit more discriminating: we will use an MLP with 3 layers to make things a bit more interesting.

```
net_D = nn.Sequential()
net_D.add(nn.Dense(5, activation='tanh'),
          nn.Dense(3, activation='tanh'),
          nn.Dense(1))
```

### 16.1.4 Training

First we define a function to update the discriminator.

```
# Save to the d2l package.
def update_D(X, Z, net_D, net_G, loss, trainer_D):
    """Update discriminator"""
    batch_size = X.shape[0]
    ones = nd.ones((batch_size,), ctx=X.context)
    zeros = nd.zeros((batch_size,), ctx=X.context)
    with autograd.record():
        real_Y = net_D(X)
        fake_X = net_G(Z)
        # Don't need to compute gradient for net_G, detach it from
        # computing gradients.
        fake_Y = net_D(fake_X.detach())
        loss_D = (loss(real_Y, ones) + loss(fake_Y, zeros)) / 2
    loss_D.backward()
    trainer_D.step(batch_size)
    return loss_D.sum().asscalar()
```

The generator is updated similarly. Here we reuse the cross-entropy loss but change the label of the fake data from 0 to 1.

```
# Save to the d2l package.
def update_G(Z, net_D, net_G, loss, trainer_G):  # saved in d2l
    """Update generator"""
    batch_size = Z.shape[0]
    ones = nd.ones((batch_size,), ctx=Z.context)
    with autograd.record():
        # We could reuse fake_X from update_D to save computation.
        fake_X = net_G(Z)
        # Recomputing fake_Y is needed since net_D is changed.
        fake_Y = net_D(fake_X)
        loss_G = loss(fake_Y, ones)
    loss_G.backward()
    trainer_G.step(batch_size)
    return loss_G.sum().asscalar()
```

Both the discriminator and the generator performs a binary logistic regression with the cross-entropy loss. We use Adam to smooth the training process. In each iteration, we first update the discriminator and then the generator. We visualize both losses and generated examples.

```

def train(net_D, net_G, data_iter, num_epochs, lr_D, lr_G, latent_dim, data):
    loss = gluon.loss.SigmoidBCELoss()
    net_D.initialize(init=init.Normal(0.02), force_reinit=True)
    net_G.initialize(init=init.Normal(0.02), force_reinit=True)
    trainer_D = gluon.Trainer(net_D.collect_params(),
                               'adam', {'learning_rate': lr_D})
    trainer_G = gluon.Trainer(net_G.collect_params(),
                               'adam', {'learning_rate': lr_G})
    animator = d2l.Animator(xlabel='epoch', ylabel='loss',
                             xlim=[1, num_epochs], nrows=2, figsize=(5,5),
                             legend=['generator', 'discriminator'])
    animator.fig.subplots_adjust(hspace=0.3)
    for epoch in range(1, num_epochs+1):
        # Train one epoch
        timer = d2l.Timer()
        metric = d2l.Accumulator(3) # loss_D, loss_G, num_examples
        for X in data_iter:
            batch_size = X.shape[0]
            Z = nd.random.normal(0, 1, shape=(batch_size, latent_dim))
            metric.add(update_D(X, Z, net_D, net_G, loss, trainer_D),
                       update_G(Z, net_D, net_G, loss, trainer_G),
                       batch_size)
        # Visualize generated examples
        Z = nd.random.normal(0, 1, shape=(100, latent_dim))
        fake_X = net_G(Z).asnumpy()
        animator.axes[1].cla()
        animator.axes[1].scatter(data[:,0], data[:,1])
        animator.axes[1].scatter(fake_X[:,0], fake_X[:,1])
        animator.axes[1].legend(['real', 'generated'])
        # Show the losses
        loss_D, loss_G = metric[0]/metric[2], metric[1]/metric[2]
        animator.add(epoch, (loss_D, loss_G))
        print('loss_D %.3f, loss_G %.3f, %d examples/sec' % (
            loss_D, loss_G, metric[2]/timer.stop())))

```

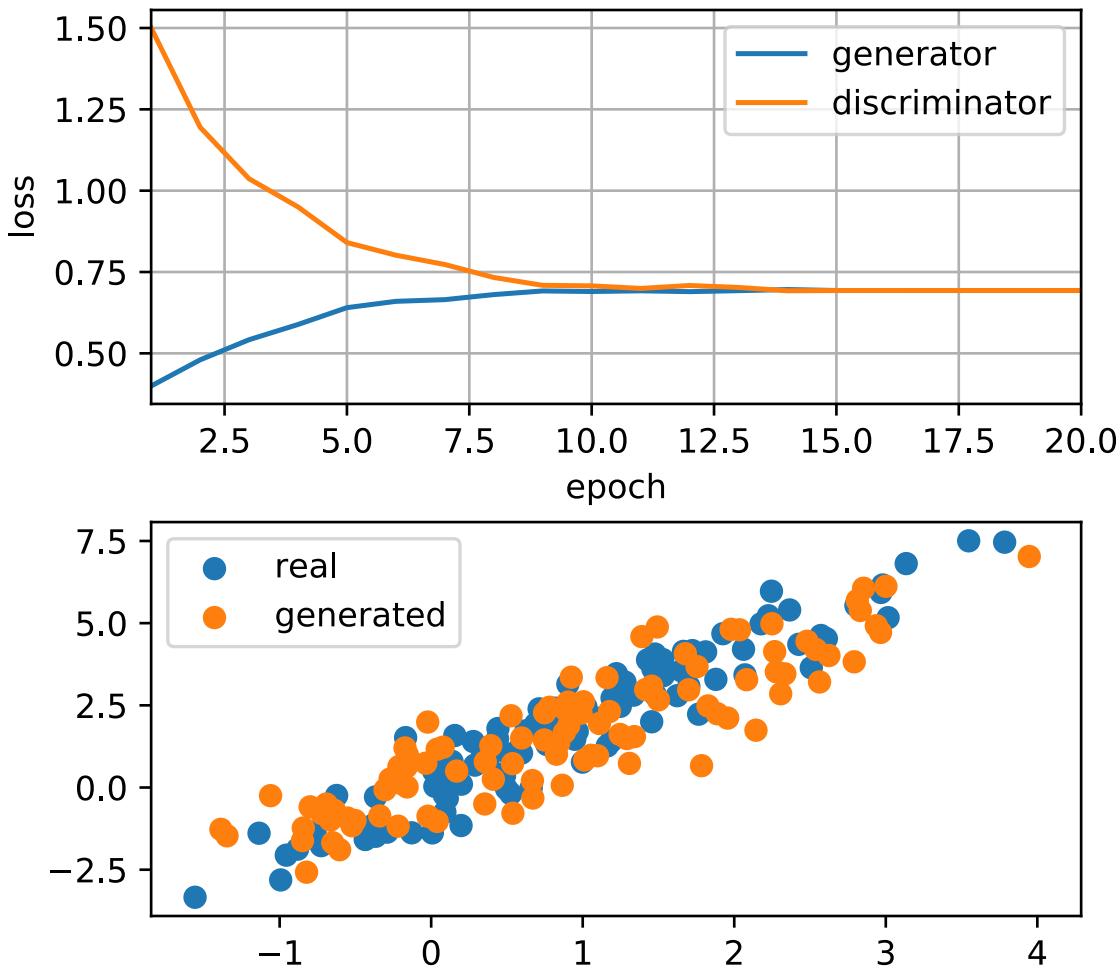
Now we specify the hyper-parameters to fit the Gaussian distribution.

```

lr_D, lr_G, latent_dim, num_epochs = 0.05, 0.005, 2, 20
train(net_D, net_G, data_iter, num_epochs, lr_D, lr_G,
      latent_dim, data[:100].asnumpy())

```

```
loss_D 0.693, loss_G 0.693, 790 examples/sec
```



### 16.1.5 Summary

- Generative adversarial networks (GANs) compose of two deep networks, the generator and the discriminator.
- The generator generates the image as much closer to the true image as possible to fool the discriminator, via maximizing the cross-entropy loss, i.e.,  $\max \log(D(\mathbf{x}'))$ .
- The discriminator tries to distinguish the generated images from the true images, via minimizing the cross-entropy loss, i.e.,  $\min -y \log D(\mathbf{x}) - (1 - y) \log(1 - D(\mathbf{x}))$ .

### 16.1.6 Reference

## 16.2 Deep Convolutional Generative Adversarial Networks

In Section 16.1, we introduced the basic ideas behind how GANs work. We showed that they can draw samples from some simple, easy-to-sample distribution, like a uniform or normal distribution, and transform them into samples that appear to match the distribution of some data set. And while our example of matching a 2D Gaussian distribution got the point across, it's not especially exciting.

In this section, we'll demonstrate how you can use GANs to generate photorealistic images. We'll be basing our models on the deep convolutional GANs (DCGAN) introduced in [49]. We'll borrow the convolutional architecture that have proven so successful for discriminative computer vision problems and show how via GANs, they can be leveraged to generate photorealistic images.

```
from mxnet import nd, gluon, autograd, init
from mxnet.gluon import nn
import d2l
import zipfile
import numpy as np
```

### 16.2.1 The Pokemon Dataset

The dataset we will use is a collection of Pokemon sprites obtained from pokemondb<sup>206</sup>. First download, extract and load this dataset.

```
data_dir = '../data/'
url = 'http://data.mxnet.io/data/pokemon.zip'
sha1 = 'c065c0e2593b8b161a2d7873e42418bf6a21106c'
fname = gluon.utils.download(url, data_dir, sha1_hash=sha1)
with zipfile.ZipFile(fname) as f:
    f.extractall(data_dir)
pokemon = gluon.data.vision.datasets.ImageFolderDataset(data_dir+'pokemon')
```

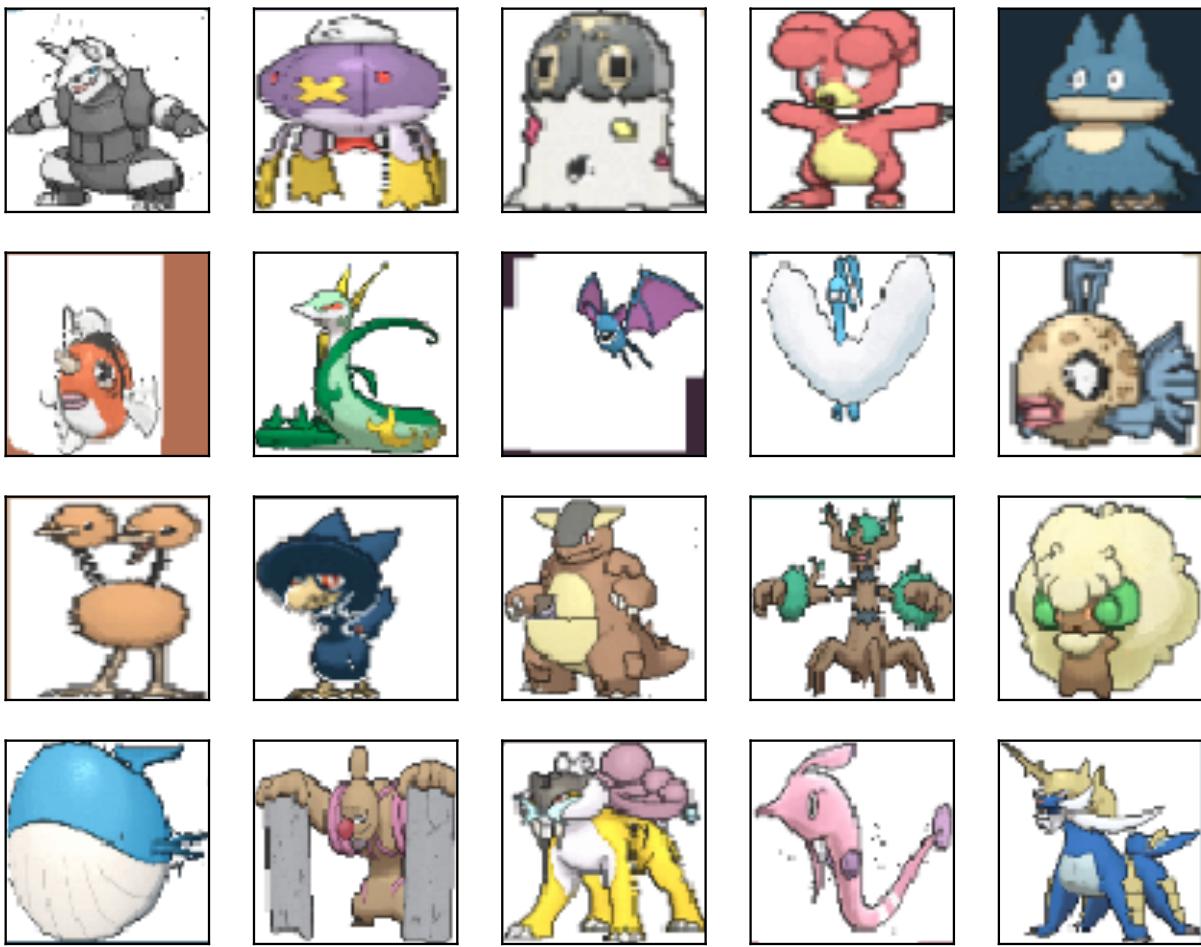
We resize each image into  $64 \times 64$ . The `ToTensor` transformation will project the pixel value into  $[0, 1]$ , while our generator will use the `tanh` function to obtain outputs in  $[-1, 1]$ . Therefore we normalize the data with 1/2 mean and 1/2 variance to match the value range.

```
batch_size = 256
transformer = gluon.data.vision.transforms.Compose([
    gluon.data.vision.transforms.Resize(64),
    gluon.data.vision.transforms.ToTensor(),
    gluon.data.vision.transforms.Normalize(0.5, 0.5)
])
data_iter = gluon.data.DataLoader(
    pokemon.transform_first(transformer), batch_size=batch_size,
    shuffle=True, num_workers=d2l.get_dataloader_workers())
```

Let's visualize the first 20 images.

```
d2l.set_figsize((4, 4))
for X, y in data_iter:
    imgs = X[0:20,:,:,:].transpose((0,2,3,1))/2+0.5
    d2l.show_images(imgs, num_rows=4, num_cols=5)
    break
```

<sup>206</sup> <https://pokemondb.net/sprites>



### 16.2.2 The Generator

The generator needs to map the noise variable  $\mathbf{z} \in \mathbb{R}^d$ , a length- $d$  vector, to a RGB image with both width and height to be 64. In Section 14.11 we introduced the fully convolutional network that uses transposed convolution layer (refer to Section 14.10) to enlarge input size. The basic block of the generator contains a transposed convolution layer followed by the batch normalization and ReLU activation.

```
class G_block(nn.Block):
    def __init__(self, channels, kernel_size=4,
                 strides=2, padding=1, **kwargs):
        super(G_block, self).__init__(**kwargs)
        self.conv2d_trans = nn.Conv2DTranspose(
            channels, kernel_size, strides, padding, use_bias=False)
        self.batch_norm = nn.BatchNorm()
        self.activation = nn.Activation('relu')

    def forward(self, X):
        return self.activation(self.batch_norm(self.conv2d_trans(X)))
```

In default, the transposed convolution layer uses a  $4 \times 4$  kernel,  $2 \times 2$  strides and  $1 \times 1$  padding. It will double input's width and height.

```
x = nd.zeros((2, 3, 16, 16))
g_blk = G_block(20)
g_blk.initialize()
g_blk(x).shape
```

```
(2, 20, 32, 32)
```

Changing strides to 1 and padding to 0 will lead to increase both input's width and height by 3.

```
x = nd.zeros((2, 3, 1, 1))
g_blk = G_block(20, strides=1, padding=0)
g_blk.initialize()
g_blk(x).shape
```

```
(2, 20, 4, 4)
```

The generator consists of four basic blocks that increase input's both width and height from 1 to 32. At the same time, it first projects the latent variable into  $64 \times 8$  channels, and then halve the channels each time. At last, a transposed convolution layer is used to generate the output. It further doubles the width and height to match the desired  $64 \times 64$  shape, and reduces the channel size to 3. The tanh activation function is applied to project output values into the  $(-1, 1)$  range.

```
n_G = 64
net_G = nn.Sequential()
net_G.add(G_block(n_G*8, strides=1, padding=0), # output: (64*8, 4, 4)
          G_block(n_G*4), # output: (64*4, 8, 8)
          G_block(n_G*2), # output: (64*2, 16, 16)
          G_block(n_G), # output: (64, 32, 32)
          nn.Conv2DTranspose(
              3, kernel_size=4, strides=2, padding=1, use_bias=False,
              activation='tanh')) # output: (3, 64, 64)
```

Generate a 100 dimensional latent variable to verify the generator's output shape.

```
x = nd.zeros((1, 100, 1, 1))
net_G.initialize()
net_G(x).shape
```

```
(1, 3, 64, 64)
```

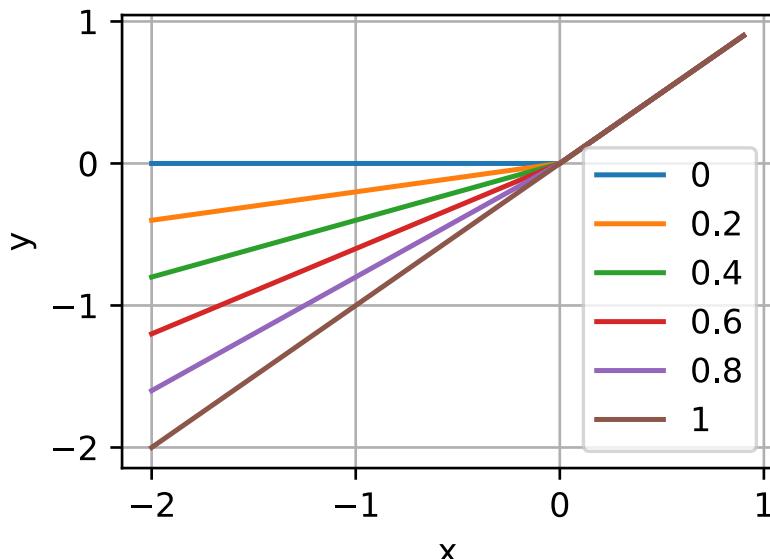
### 16.2.3 Discriminator

The discriminator is a normal convolutional network network except that it uses a leaky ReLU as its activation function. Given  $\alpha \in [0, 1]$ , its definition is

$$\text{leaky ReLU}(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha x & \text{otherwise} \end{cases}. \quad (16.2.1)$$

As it can be seen, it is normal ReLU if  $\alpha = 0$ , and an identity function if  $\alpha = 1$ . For  $\alpha \in (0, 1)$ , leaky ReLU is a nonlinear function that give a non-zero output for a negative input. It aims to fix the “dying ReLU” problem that a neuron might always output a negative value and therefore cannot make any progress since the gradient of ReLU is 0.

```
alphas = [0, 0.2, 0.4, .6, .8, 1]
x = nd.arange(-2, 1, 0.1)
Y = [nn.LeakyReLU(alpha)(x).asnumpy() for alpha in alphas]
d2l.plot(x.asnumpy(), Y, 'x', 'y', alphas)
```



The basic block of the discriminator is a convolution layer followed by a batch normalization layer and a leaky ReLU activation. The hyper-parameters of the convolution layer are similar to the transpose convolution layer in the generator block.

```
class D_block(nn.Block):
    def __init__(self, channels, kernel_size=4, strides=2,
                 padding=1, alpha=0.2, **kwargs):
        super(D_block, self).__init__(**kwargs)
        self.conv2d = nn.Conv2D(
            channels, kernel_size, strides, padding, use_bias=False)
        self.batch_norm = nn.BatchNorm()
        self.activation = nn.LeakyReLU(alpha)

    def forward(self, X):
        return self.activation(self.batch_norm(self.conv2d(X)))
```

A basic block will halve the width and height of the inputs.

```
x = nd.zeros((2, 3, 16, 16))
d_blk = D_block(20)
d_blk.initialize()
d_blk(x).shape
```

```
(2, 20, 8, 8)
```

The discriminator is a mirror of the generator.

```
n_D = 64
net_D = nn.Sequential()
net_D.add(D_block(n_D),      # output: (64, 32, 32)
          D_block(n_D*2),    # output: (64*2, 16, 16)
          D_block(n_D*4),    # output: (64*4, 8, 8)
          D_block(n_D*8),    # output: (64*8, 4, 4)
          nn.Conv2D(1, kernel_size=4, use_bias=False))  # output: (1, 1, 1)
```

It uses a convolution layer with output channel 1 as the last layer to obtain a single prediction value.

```
x = nd.zeros((1, 3, 64, 64))
net_D.initialize()
net_D(x).shape
```

```
(1, 1, 1, 1)
```

#### 16.2.4 Training

Compared to the basic GAN in Section 16.1, we use the same learning rate for both generator and discriminator since they are similar to each other. In addition, we change  $\beta_1$  in Adam (Section 12.10) from 0.9 to 0.5. It decreases the smoothness of the momentum, the exponentially weighted moving average of past gradients, to take care of the rapid changing gradients because the generator and the discriminator fight with each other. Besides, Z is a 4-D tensor and we are using GPU to accelerate the computation.

```
def train(net_D, net_G, data_iter, num_epochs, lr, latent_dim,
          ctx=d2l.try_gpu()):
    loss = gluon.loss.SigmoidBCELoss()
    net_D.initialize(init=init.Normal(0.02), force_reinit=True, ctx=ctx)
    net_G.initialize(init=init.Normal(0.02), force_reinit=True, ctx=ctx)
    trainer_hp = {'learning_rate': lr, 'beta1': 0.5}
    trainer_D = gluon.Trainer(net_D.collect_params(), 'adam', trainer_hp)
    trainer_G = gluon.Trainer(net_G.collect_params(), 'adam', trainer_hp)
    animator = d2l.Animator(xlabel='epoch', ylabel='loss',
                             xlim=[1, num_epochs], nrows=2, figsize=(5,5),
                             legend=['generator', 'discriminator'])
    animator.fig.subplots_adjust(hspace=0.3)
    for epoch in range(1, num_epochs+1):
        # Train one epoch
        timer = d2l.Timer()
        metric = d2l.Accumulator(3)  # loss_D, loss_G, num_examples
        for X, _ in data_iter:
            batch_size = X.shape[0]
            Z = nd.random.normal(0, 1, shape=(batch_size, latent_dim, 1, 1))
            X, Z = X.as_in_context(ctx), Z.as_in_context(ctx),
            metric.add(d2l.update_D(X, Z, net_D, net_G, loss, trainer_D),
                       d2l.update_G(Z, net_D, net_G, loss, trainer_G),
                       batch_size)
        # Show generated examples
        Z = nd.random.normal(0, 1, shape=(21, latent_dim, 1, 1), ctx=ctx)
        fake_x = (net_G(Z).transpose((0,2,3,1))/2+0.5).asnumpy()
        imgs = np.vstack([np.hstack(fake_x[i:i+7])]
```

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```

        for i in range(0, len(fake_x), 7)):
    animator.axes[1].cla()
    animator.axes[1].imshow(imgs)
    # Show the losses
    loss_D, loss_G = metric[0]/metric[2], metric[1]/metric[2]
    animator.add(epoch, (loss_D, loss_G))
    print('loss_D %.3f, loss_G %.3f, %d examples/sec on %s' %
          (loss_D, loss_G, metric[2]/timer.stop(), ctx))

```

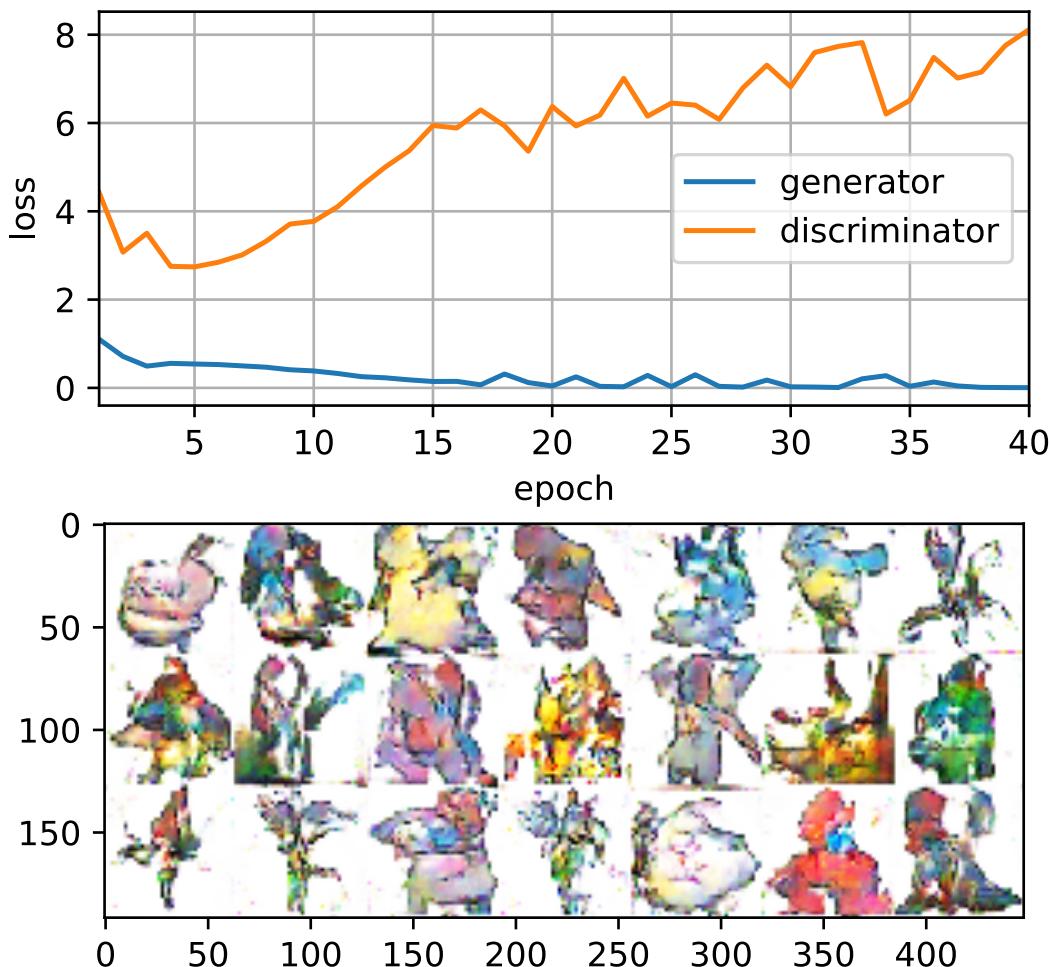
Now let's train the model.

```

latent_dim, lr, num_epochs = 100, 0.005, 40
train(net_D, net_G, data_iter, num_epochs, lr, latent_dim)

```

```
loss_D 0.005, loss_G 8.117, 2607 examples/sec on gpu(0)
```



### 16.2.5 Summary

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CHAPTER  
SEVENTEEN

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APPENDIX

## 17.1 List of Main Symbols

The main symbols used in this book are listed below.

### 17.1.1 Numbers

Symbol	Type
$x$	Scalar
$\mathbf{x}$	Vector
$\mathbf{X}$	Matrix
$\mathbf{X}$	Tensor

### 17.1.2 Sets

Symbol	Type
$\mathcal{X}$	Set
$\mathbb{R}$	Real numbers
$\mathbb{R}^n$	Vectors of real numbers in $n$ dimensions
$\mathbb{R}^{a \times b}$	Matrix of real numbers with $a$ rows and $b$ columns

### 17.1.3 Operators

Symbol	Type
$(\cdot)^\top$	Vector or matrix transposition
$\odot$	Element-wise multiplication
$ \mathcal{X} $	Cardinality (number of elements) of the set $\mathcal{X}$
$\ \cdot\ _p$	$L_p$ norm
$\ \cdot\ $	$L_2$ norm
$\sum$	Series addition
$\prod$	Series multiplication

### 17.1.4 Functions

Symbol	Type
$f(\cdot)$	Function
$\log(\cdot)$	Natural logarithm
$\exp(\cdot)$	Exponential function

### 17.1.5 Derivatives and Gradients

Symbol	Type
$\frac{dy}{dx}$	Derivative of $y$ with respect to $x$
$\partial_{xy}$	Partial derivative of $y$ with respect to $x$
$\nabla_{\mathbf{x}}y$	Gradient of $y$ with respect to $\mathbf{x}$

### 17.1.6 Probability and Statistics

Symbol	Type
$\Pr(\cdot)$	Probability distribution
$z \sim \Pr$	Random variable $z$ obeys the probability distribution $\Pr$
$\Pr(x y)$	Conditional probability of $x y$
$\mathbf{E}_x[f(x)]$	Expectation of $f$ with respect to $x$

### 17.1.7 Complexity

Symbol	Type
$\mathcal{O}$	Big O notation
$\mathcal{o}$	Little o notation (grows much more slowly than)

## 17.2 Mathematical Basics

This section summarizes basic tools from linear algebra, differentiation, and probability required to understand the contents in this book. We avoid details beyond the bare minimum to keep things streamlined and easily accessible. In some cases we simplify things to keep them easily accessible. For more background see e.g. the excellent [Data Science 100](#)<sup>207</sup> course at UC Berkeley.

### 17.2.1 Linear Algebra

This is a brief summary of vectors, matrices, operators, norms, eigenvectors, and eigenvalues. They're needed since a significant part of deep learning revolves around manipulating matrices and vectors. For a much more in-depth introduction to linear algebra in Python see e.g. the [Jupyter notebooks](#)<sup>208</sup> of Gilbert Strang's MIT course on [Linear Algebra](#)<sup>209</sup>.

<sup>207</sup> <http://ds100.org>

<sup>208</sup> [https://github.com/juanklopper/MIT\\_OCW\\_Linear\\_Algebra\\_18\\_06](https://github.com/juanklopper/MIT_OCW_Linear_Algebra_18_06)

<sup>209</sup> <http://web.mit.edu/18.06/www/videos.shtml>

## Vectors

By default we refer to column vectors in this book. An  $n$ -dimensional vector  $\mathbf{x}$  can be written as

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}. \quad (17.2.1)$$

Here  $x_1, \dots, x_n$  are elements of the vector. To express that  $\mathbf{x}$  is an  $n$ -dimensional vector with elements from the set of real numbers, we write  $\mathbf{x} \in \mathbb{R}^n$  or  $\mathbf{x} \in \mathbb{R}^{n \times 1}$ . Vectors satisfy the basic operations of a *vector space*, namely that you can add them together and multiply them with scalars (in our case element-wise) and you still get a vector back: assuming that  $\mathbf{a}, \mathbf{b} \in \mathbb{R}^n$  and  $\alpha \in \mathbb{R}$  we have that  $\mathbf{a} + \mathbf{b} \in \mathbb{R}^n$  and  $\alpha \cdot \mathbf{a} \in \mathbb{R}^n$ . Furthermore they satisfy the distributive law

$$\alpha \cdot (\mathbf{a} + \mathbf{b}) = \alpha \cdot \mathbf{a} + \alpha \cdot \mathbf{b}. \quad (17.2.2)$$

## Matrices

A matrix with  $m$  rows and  $n$  columns can be written as

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1n} \\ x_{21} & x_{22} & \dots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \dots & x_{mn} \end{bmatrix}. \quad (17.2.3)$$

Here,  $x_{ij}$  is the element in row  $i \in \{1, \dots, m\}$  and column  $j \in \{1, \dots, n\}$  in the matrix  $\mathbf{X}$ . Extending the vector notation we use  $\mathbf{X} \in \mathbb{R}^{m \times n}$  to indicate that  $\mathbf{X}$  is an  $m \times n$  matrix. Given the above we could interpret vectors as  $m \times 1$  dimensional matrices. Furthermore, matrices also form a vector space, i.e. we can multiply and add them just fine, as long as their dimensions match.

## Operations

Assume that the elements in the  $\mathbf{a}, \mathbf{b} \in \mathbb{R}^n$  are  $a_1, \dots, a_n$  and  $b_1, \dots, b_n$  respectively. The dot product (internal product) of vectors  $\mathbf{a}$  and  $\mathbf{b}$  is a scalar:

$$\mathbf{a} \cdot \mathbf{b} = a_1 b_1 + \dots + a_n b_n. \quad (17.2.4)$$

Assume that we have two matrices with  $m$  rows and  $n$  columns  $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{m \times n}$ :

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} b_{11} & b_{12} & \dots & b_{1n} \\ b_{21} & b_{22} & \dots & b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ b_{m1} & b_{m2} & \dots & b_{mn} \end{bmatrix}. \quad (17.2.5)$$

The transpose of a matrix  $\mathbf{A}^\top \in \mathbb{R}^{n \times m}$  is a matrix with  $n$  rows and  $m$  columns which are formed by “flipping” over the original matrix as follows:

$$\mathbf{A}^\top = \begin{bmatrix} a_{11} & a_{21} & \dots & a_{m1} \\ a_{12} & a_{22} & \dots & a_{m2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1n} & a_{2n} & \dots & a_{mn} \end{bmatrix} \quad (17.2.6)$$

To add two matrices of the same shape, we add them element-wise:

$$\mathbf{A} + \mathbf{B} = \begin{bmatrix} a_{11} + b_{11} & a_{12} + b_{12} & \dots & a_{1n} + b_{1n} \\ a_{21} + b_{21} & a_{22} + b_{22} & \dots & a_{2n} + b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} + b_{m1} & a_{m2} + b_{m2} & \dots & a_{mn} + b_{mn} \end{bmatrix}. \quad (17.2.7)$$

We use the symbol  $\odot$  to indicate the element-wise multiplication of two matrices (in Matlab notation this is `.*`):

$$\mathbf{A} \odot \mathbf{B} = \begin{bmatrix} a_{11}b_{11} & a_{12}b_{12} & \dots & a_{1n}b_{1n} \\ a_{21}b_{21} & a_{22}b_{22} & \dots & a_{2n}b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}b_{m1} & a_{m2}b_{m2} & \dots & a_{mn}b_{mn} \end{bmatrix}. \quad (17.2.8)$$

Define a scalar  $k$ . Multiplication of scalars and matrices is also an element-wise multiplication:

$$k \cdot \mathbf{A} = \begin{bmatrix} ka_{11} & ka_{12} & \dots & ka_{1n} \\ ka_{21} & ka_{22} & \dots & ka_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ ka_{m1} & ka_{m2} & \dots & ka_{mn} \end{bmatrix}. \quad (17.2.9)$$

Other operations such as scalar and matrix addition, and division by an element are similar to the multiplication operation in the above equation. Calculating the square root or taking logarithms of a matrix are performed by calculating the square root or logarithm, respectively, of each element of the matrix to obtain a matrix with the same shape as the original matrix.

Matrix multiplication is different from element-wise matrix multiplication. Assume  $\mathbf{A}$  is a matrix with  $m$  rows and  $p$  columns and  $\mathbf{B}$  is a matrix with  $p$  rows and  $n$  columns. The product (matrix multiplication) of these two matrices is denoted as

$$\mathbf{AB} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1p} \\ a_{21} & a_{22} & \dots & a_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{i1} & a_{i2} & \dots & a_{ip} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mp} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & \dots & b_{1j} & \dots & b_{1n} \\ b_{21} & b_{22} & \dots & b_{2j} & \dots & b_{2n} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ b_{p1} & b_{p2} & \dots & b_{pj} & \dots & b_{pn} \end{bmatrix}. \quad (17.2.10)$$

The product is a matrix with  $m$  rows and  $n$  columns, with the element in row  $i \in \{1, \dots, m\}$  and column  $j \in \{1, \dots, n\}$  equal to

$$[\mathbf{AB}]_{ij} = a_{i1}b_{1j} + a_{i2}b_{2j} + \dots + a_{ip}b_{pj} = \sum_{k=1}^p a_{ik}b_{kj}. \quad (17.2.11)$$

## Norms

Assume that the elements in the  $n$ -dimensional vector  $\mathbf{x}$  are  $x_1, \dots, x_n$ . The  $\ell_p$  norm of  $\mathbf{x}$  is

$$\|\mathbf{x}\|_p = \left( \sum_{i=1}^n |x_i|^p \right)^{1/p}. \quad (17.2.12)$$

For example, the  $\ell_1$  norm of  $\mathbf{x}$  is the sum of the absolute values of the vector elements:

$$\|\mathbf{x}\|_1 = \sum_{i=1}^n |x_i|. \quad (17.2.13)$$

The  $\ell_2$  norm of  $\mathbf{x}$  is the square root of the sum of the squares of the vector elements:

$$\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^n x_i^2}. \quad (17.2.14)$$

We usually use  $\|\mathbf{x}\|$  to refer to the  $\ell_2$  norm of  $\mathbf{x}$ . Lastly, the  $\ell_\infty$  norm of a vector is the limit of the above definition. This works out to

$$\|\mathbf{x}\|_\infty = \max_i |x_i|. \quad (17.2.15)$$

Assume  $\mathbf{X}$  is a matrix with  $m$  rows and  $n$  columns. The Frobenius norm of matrix  $\mathbf{X}$  is the square root of the sum of the squares of the matrix elements:

$$\|\mathbf{X}\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n x_{ij}^2}. \quad (17.2.16)$$

Here,  $x_{ij}$  is the element of matrix  $\mathbf{X}$  in row  $i$  and column  $j$ . In other words, the Frobenius norm behaves as if it were an  $\ell_2$  norm of a matrix-shaped vector.

**Note:** sometimes the norms on vectors are also (erroneously) referred to as  $L_p$  norms. However, the latter are norms on functions with similar structure. For instance, the  $L_2$  norm of a function  $f$  is given by  $\|f\|_2^2 = \int |f(x)|^2 dx$ .

## Eigenvectors and Eigenvalues

Let  $\mathbf{A}$  be a matrix with  $n$  rows and  $n$  columns. If  $\lambda$  is a scalar and  $\mathbf{v}$  is a non-zero  $n$ -dimensional vector with

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}, \quad (17.2.17)$$

then  $\mathbf{v}$  is called an eigenvector of matrix  $\mathbf{A}$  and  $\lambda$  is called an eigenvalue of  $\mathbf{A}$  corresponding to  $\mathbf{v}$ . For symmetric matrices  $\mathbf{A} = \mathbf{A}^\top$  there are exactly  $n$  (linearly independent) eigenvector and eigenvalue pairs.

## 17.2.2 Differentials

This is a very brief primer on multivariate differential calculus.

### Derivatives and Differentials

Assume the input and output of function  $f : \mathbb{R} \rightarrow \mathbb{R}$  are both scalars. The derivative  $f'$  is defined as

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}, \quad (17.2.18)$$

when the limit exists (and  $f$  is said to be differentiable). Given  $y = f(x)$ , where  $x$  and  $y$  are the arguments and dependent variables of function  $f$ , respectively, the following derivative and differential expressions are equivalent:

$$f'(x) = y' = \frac{dy}{dx} = \frac{df}{dx} = \frac{d}{dx} f(x) = Df(x) = D_x f(x), \quad (17.2.19)$$

Here, the symbols  $D$  and  $\frac{d}{dx}$  are also called differential operators. Common differential calculations are  $DC = 0$  ( $C$  is a constant),  $Dx^n = nx^{n-1}$  ( $n$  is a constant),  $D e^x = e^x$ , and  $D \ln(x) = 1/x$ .

If functions  $f$  and  $g$  are both differentiable and  $C$  is a constant, then

$$\begin{aligned}\frac{d}{dx}[Cf(x)] &= C\frac{d}{dx}f(x), \\ \frac{d}{dx}[f(x) + g(x)] &= \frac{d}{dx}f(x) + \frac{d}{dx}g(x), \\ \frac{d}{dx}[f(x)g(x)] &= f(x)\frac{d}{dx}[g(x)] + g(x)\frac{d}{dx}[f(x)], \\ \frac{d}{dx}\left[\frac{f(x)}{g(x)}\right] &= \frac{g(x)\frac{d}{dx}[f(x)] - f(x)\frac{d}{dx}[g(x)]}{[g(x)]^2}.\end{aligned}\tag{17.2.20}$$

If functions  $y = f(u)$  and  $u = g(x)$  are both differentiable, then the chain rule states that

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx}.\tag{17.2.21}$$

## Taylor Expansion

The Taylor expansion of function  $f$  is given by the infinite sum

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n,\tag{17.2.22}$$

if it exists. Here,  $f^{(n)}$  is the  $n$ th derivative of  $f$ , and  $n!$  is the factorial of  $n$ . For a sufficiently small number  $\epsilon$ , we can replace  $x$  and  $a$  with  $x + \epsilon$  and  $x$  respectively to obtain

$$f(x + \epsilon) \approx f(x) + f'(x)\epsilon + \mathcal{O}(\epsilon^2).\tag{17.2.23}$$

Because  $\epsilon$  is sufficiently small, the above formula can be simplified to

$$f(x + \epsilon) \approx f(x) + f'(x)\epsilon.\tag{17.2.24}$$

## Partial Derivatives

Let  $u = f(x_1, x_2, \dots, x_n)$  be a function with  $n$  arguments. The partial derivative of  $u$  with respect to its  $i$ th parameter  $x_i$  is

$$\frac{\partial u}{\partial x_i} = \lim_{h \rightarrow 0} \frac{f(x_1, \dots, x_{i-1}, x_i + h, x_{i+1}, \dots, x_n) - f(x_1, \dots, x_i, \dots, x_n)}{h}.\tag{17.2.25}$$

The following partial derivative expressions are equivalent:

$$\frac{\partial u}{\partial x_i} = \frac{\partial f}{\partial x_i} = f_{x_i} = f_i = D_i f = D_{x_i} f.\tag{17.2.26}$$

To calculate  $\partial u / \partial x_i$ , we simply treat  $x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n$  as constants and calculate the derivative of  $u$  with respect to  $x_i$ .

## Gradients

Assume 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 function  $f(\mathbf{x})$  with respect to  $\mathbf{x}$  is a vector of  $n$  partial derivatives:

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \left[ \frac{\partial f(\mathbf{x})}{\partial x_1}, \frac{\partial f(\mathbf{x})}{\partial x_2}, \dots, \frac{\partial f(\mathbf{x})}{\partial x_n} \right]^\top.\tag{17.2.27}$$

To be concise, we sometimes use  $\nabla f(\mathbf{x})$  to replace  $\nabla_{\mathbf{x}}f(\mathbf{x})$ .

If  $\mathbf{A}$  is a matrix with  $m$  rows and  $n$  columns, and  $\mathbf{x}$  is an  $n$ -dimensional vector, the following identities hold:

$$\begin{aligned}\nabla_{\mathbf{x}} \mathbf{A} \mathbf{x} &= \mathbf{A}^\top, \\ \nabla_{\mathbf{x}} \mathbf{x}^\top \mathbf{A} &= \mathbf{A}, \\ \nabla_{\mathbf{x}} \mathbf{x}^\top \mathbf{A} \mathbf{x} &= (\mathbf{A} + \mathbf{A}^\top) \mathbf{x}, \\ \nabla_{\mathbf{x}} \|\mathbf{x}\|^2 &= \nabla_{\mathbf{x}} \mathbf{x}^\top \mathbf{x} = 2\mathbf{x}.\end{aligned}\tag{17.2.28}$$

Similarly if  $\mathbf{X}$  is a matrix, then

$$\nabla_{\mathbf{X}} \|\mathbf{X}\|_F^2 = 2\mathbf{X}.\tag{17.2.29}$$

### Hessian Matrices

Assume 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. If all second-order partial derivatives of function  $f$  exist and are continuous, then the Hessian matrix  $\mathbf{H}$  of  $f$  is a  $n \times n$  square matrix given by

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}.\tag{17.2.30}$$

Here, the second-order partial derivative is evaluated

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial}{\partial x_i} \left( \frac{\partial f}{\partial x_j} \right).\tag{17.2.31}$$

### 17.2.3 Probability

Finally, we will briefly introduce conditional probability, expectation and variance.

#### Conditional Probability

We will denote the probability of event  $A$  and event  $B$  as  $\Pr(A)$  and  $\Pr(B)$ , respectively. The probability of the simultaneous occurrence of the two events is denoted as  $\Pr(A \cap B)$  or  $\Pr(A, B)$ . In the figure above it is the shaded area. If  $B$  has non-zero probability, the conditional probability of event  $A$  given that  $B$  has occurred is

$$\Pr(A|B) = \frac{\Pr(A \cap B)}{\Pr(B)}.\tag{17.2.32}$$

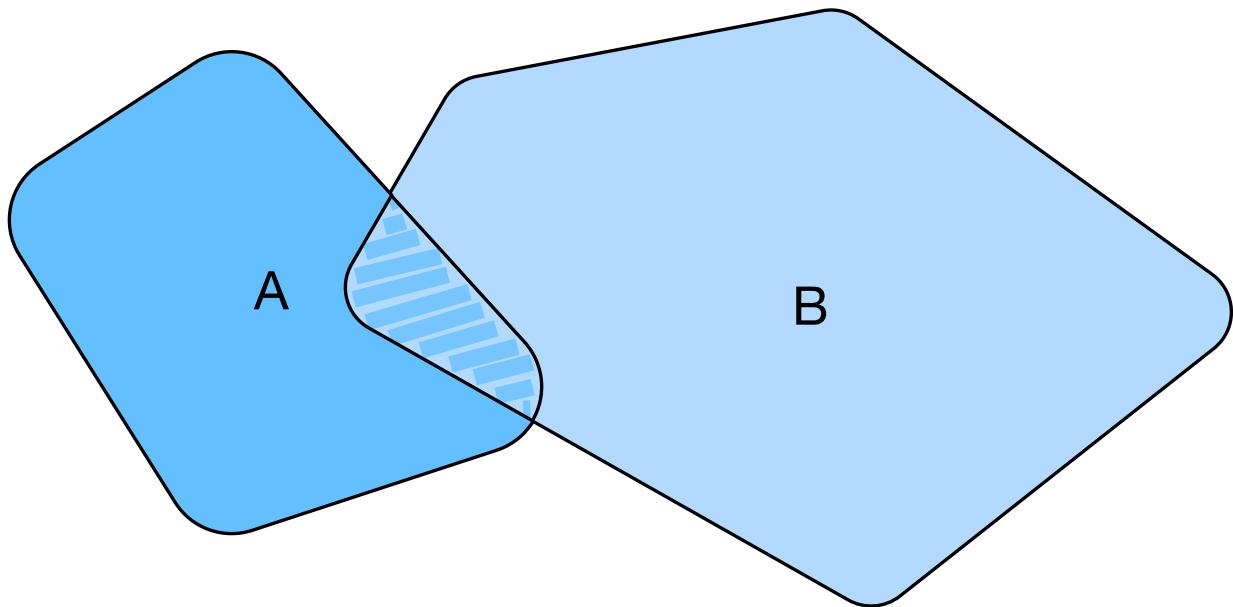
That is,

$$\Pr(A \cap B) = \Pr(B) \Pr(A|B) = \Pr(A) \Pr(B|A).\tag{17.2.33}$$

If

$$\Pr(A \cap B) = \Pr(A) \Pr(B),\tag{17.2.34}$$

then  $A$  and  $B$  are said to be independent of each other.

Fig. 17.2.1: Intersection between  $A$  and  $B$ 

### Expectation and Variance

A random variable takes values that represent possible outcomes of an experiment. The expectation (or average) of the random variable  $X$  is denoted as

$$\mathbf{E}[X] = \sum_x x \Pr(X = x). \quad (17.2.35)$$

In many cases we want to measure by how much the random variable  $x$  deviates from its expectation. This can be quantified by the variance

$$\text{Var}[X] = \mathbf{E}[(X - \mathbf{E}[X])^2] = \mathbf{E}[X^2] - \mathbf{E}^2[X]. \quad (17.2.36)$$

Here the last equality follows from the linearity of expectation.

### Uniform Distribution

Assume random variable  $X$  obeys a uniform distribution over  $[a, b]$ , i.e.  $X \sim U(a, b)$ . In this case, random variable  $X$  has the same probability of being any number between  $a$  and  $b$ .

### Normal Distribution

The Normal Distribution, also called Gaussian is given by  $p(x) = \frac{1}{2\pi\sigma^2} \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right)$ . Its expectation is  $\mu$  and its variance is  $\sigma^2$ . For more details on probability and statistics see [Section 4.4](#).

## 17.2.4 Summary

- Vectors and matrices can be added and multiplied with rules similar to those of scalars.
- There are specialized norms for vectors and matrices, quite different from the (Euclidean)  $\ell_2$  norm.
- Derivatives yield vectors and matrices when computing higher order terms.

### 17.2.5 Exercises

1. 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?
2. A square matrix is called antisymmetric if  $\mathbf{A} = -\mathbf{A}^\top$ . Show that you can decompose any square matrix into a symmetric and an antisymmetric matrix.
3. Write out a permutation in matrix form.
4. Find the gradient of the function  $f(\mathbf{x}) = 3x_1^2 + 5e^{x_2}$ .
5. What is the gradient of the function  $f(\mathbf{x}) = \|\mathbf{x}\|_2$ ?
6. Prove that  $\Pr(A \cup B) \leq \Pr(A) + \Pr(B)$ . When do you have an equality?

### 17.2.6 Scan the QR Code to Discuss<sup>210</sup>



## 17.3 Using Jupyter

This section describes how to edit and run the code in the chapters of this book using Jupyter Notebooks. Make sure you have Jupyter installed and downloaded the code as described in [Installation](#) (page 7). If you want to know more about Jupyter see the excellent tutorial in the [Documentation](#)<sup>211</sup>.

### 17.3.1 Edit and Run the Code Locally

Suppose that the local path of code of the book is “xx/yy/d2l-en/”. Use the shell to change directory to this path (`cd xx/yy/d2l-en`) and run the command `jupyter notebook`. If your browser doesn’t do this automatically, open <http://localhost:8888> and you will see the interface of Jupyter and all the folders containing the code of the book, as shown in Fig. 17.3.1.

You can access the notebook files by clicking on the folder displayed on the webpage. They usually have the suffix `.ipynb`. For the sake of brevity, we create a temporary `test.ipynb` file. The content displayed after you click it is as shown in Fig. 17.3.2. This notebook includes a markdown cell and a code cell. The content in the markdown cell includes “This is A Title” and “This is text”. The code cell contains two lines of Python code.

Double click on the markdown cell to enter edit mode. Add a new text string “Hello world.” at the end of the cell, as shown in Fig. 17.3.3.

As shown in Fig. 17.3.4, click “Cell” → “Run Cells” in the menu bar to run the edited cell.

After running, the markdown cell is as shown in Fig. 17.3.5.

Next, click on the code cell. Multiply the elements by 2 after the last line of code, as shown in Fig. 17.3.6.

<sup>210</sup> <https://discuss.mxnet.io/t/2397>

<sup>211</sup> <https://jupyter.readthedocs.io/en/latest/>

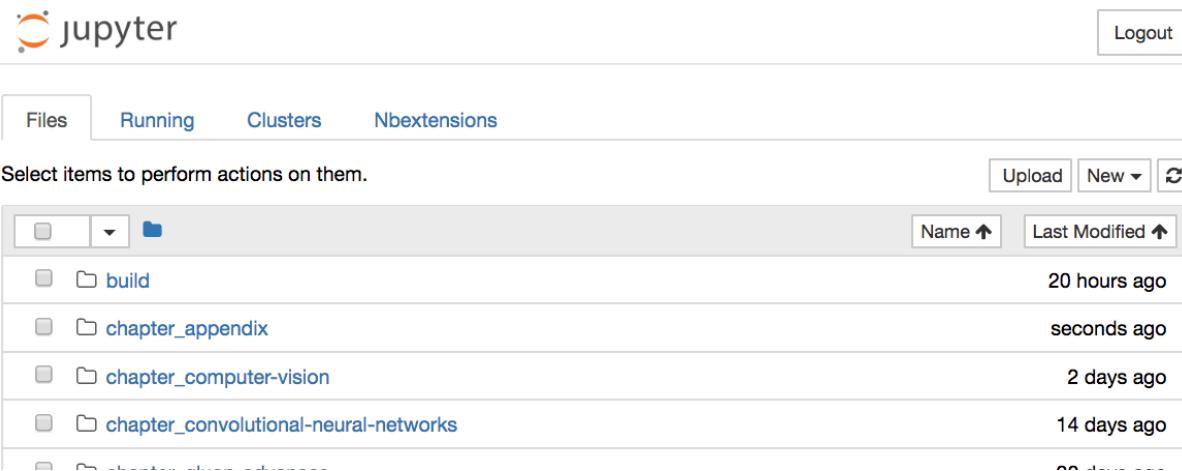


Fig. 17.3.1: The folders containing the code in this book.

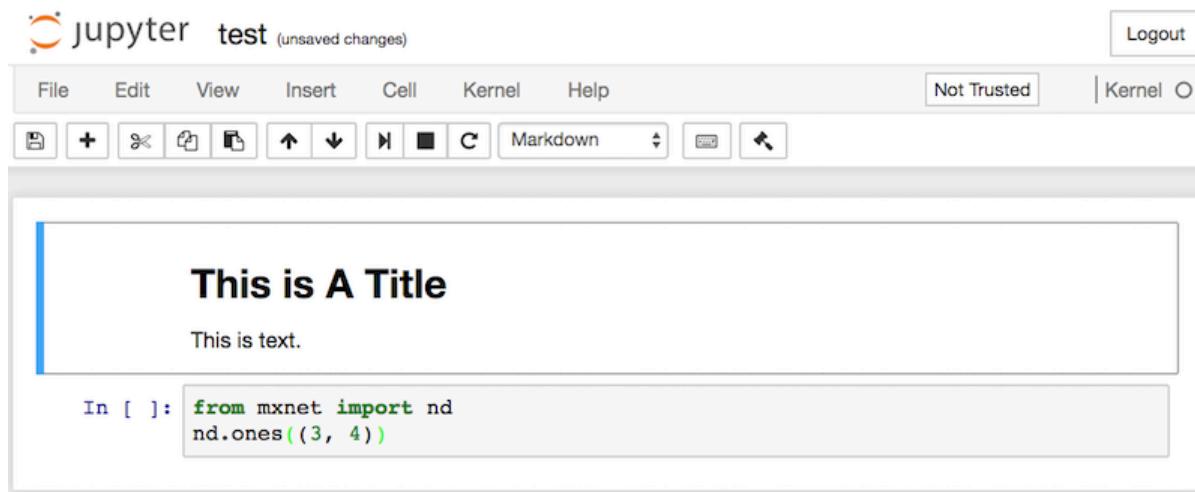


Fig. 17.3.2: Markdown and code cells in the “text.ipynb” file.

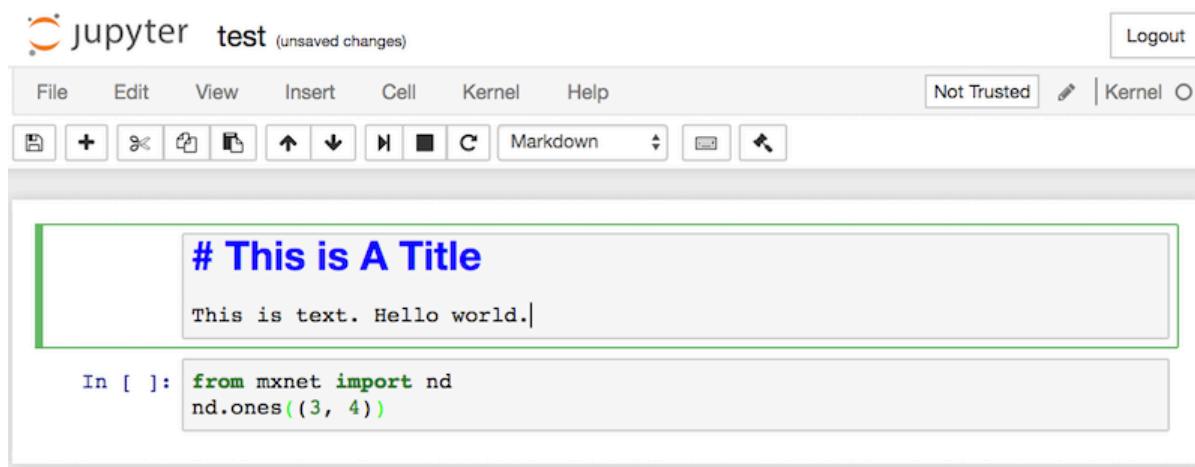


Fig. 17.3.3: Edit the markdown cell.

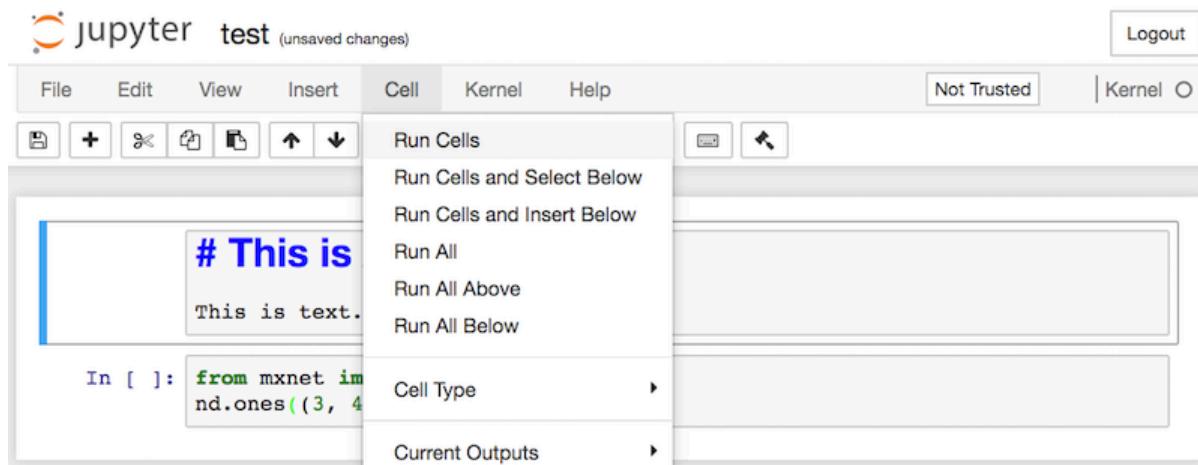


Fig. 17.3.4: Run the cell.

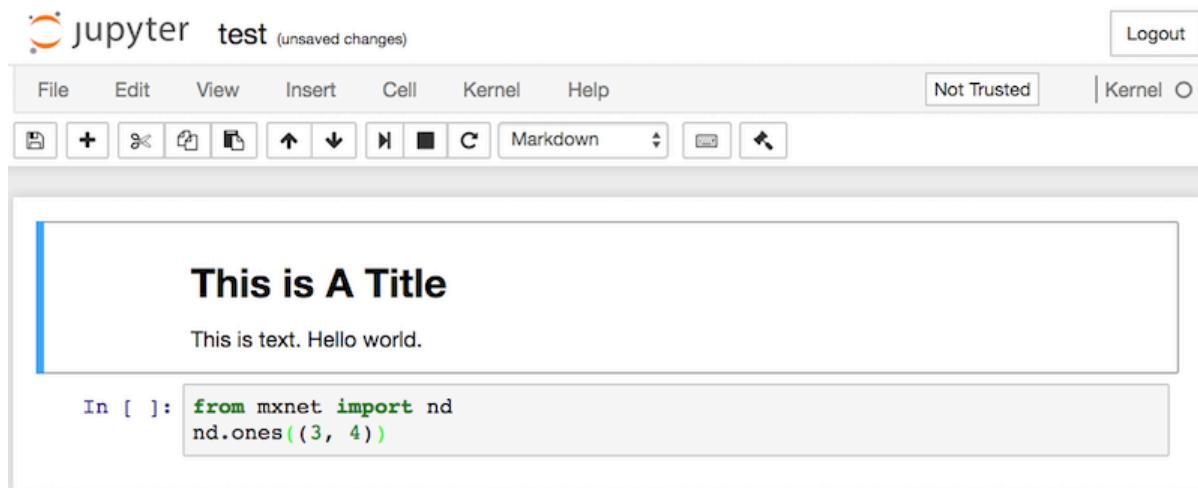


Fig. 17.3.5: The markdown cell after editing.

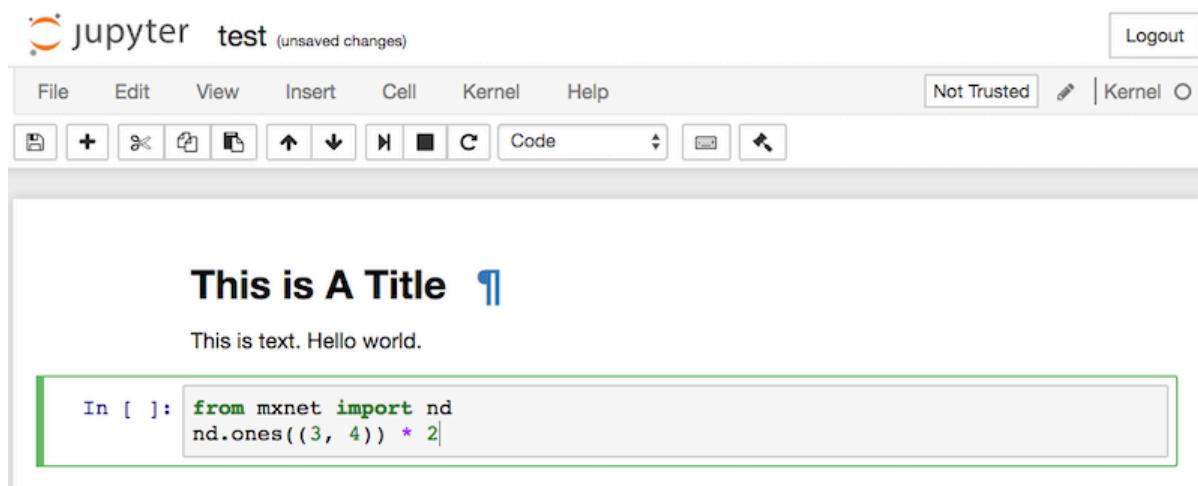


Fig. 17.3.6: Edit the code cell.

You can also run the cell with a shortcut (“Ctrl + Enter” by default) and obtain the output result from Fig. 17.3.7.

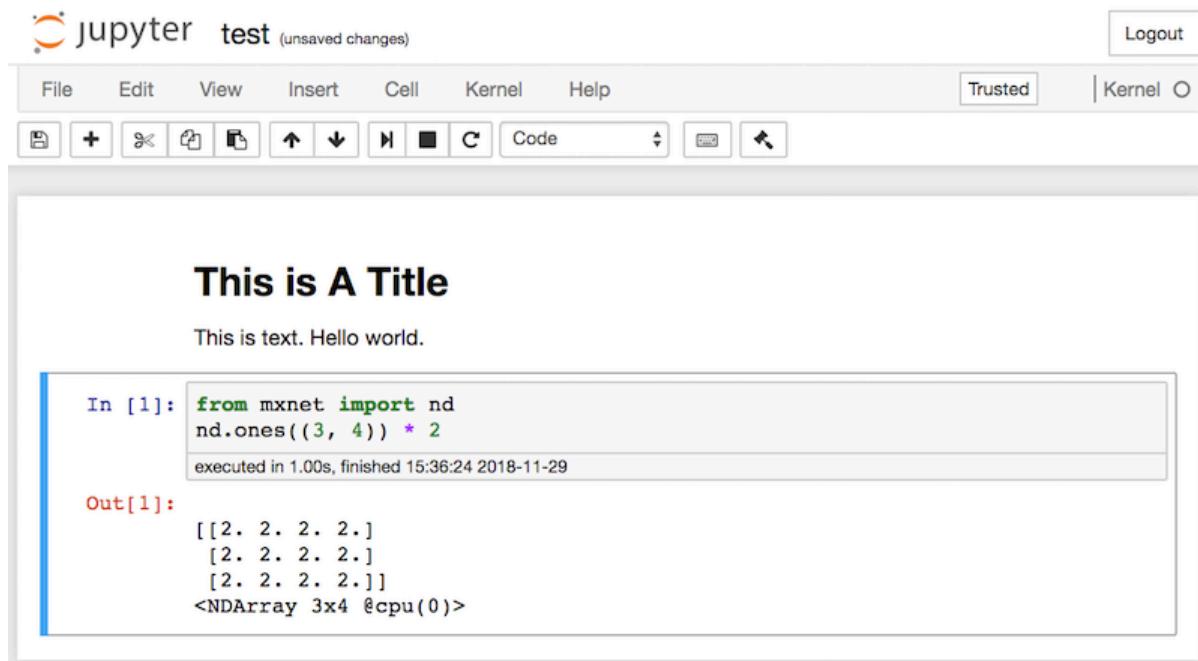


Fig. 17.3.7: Run the code cell to obtain the output.

When a notebook contains more cells, we can click “Kernel” → “Restart & Run All” in the menu bar to run all the cells in the entire notebook. By clicking “Help” → “Edit Keyboard Shortcuts” in the menu bar, you can edit the shortcuts according to your preferences.

### 17.3.2 Advanced Options

Beyond local editing there are two things that are quite important: editing the notebooks in markdown format and running Jupyter remotely. The latter matters when we want to run the code on a faster server. The former matters since Jupyter’s native .ipynb format stores a lot of auxiliary data that isn’t really specific to what is in the notebooks, mostly related to how and where the code is run. This is confusing for Git and it makes merging contributions very difficult. Fortunately there’s an alternative - native editing in Markdown.

#### Markdown Files in Jupyter

If you wish to contribute to the content of this book, you need to modify the source file (.md file, not .ipynb file) on GitHub. Using the notedown plugin we can modify notebooks in .md format directly in Jupyter.

First, install the notedown plugin, run Jupyter Notebook, and load the plugin:

```
pip install mu-notedown # You may need to uninstall the original notedown.\njupyter notebook --NotebookApp.contents_manager_class='notedown.NotedownContentsManager'
```

To turn on the notedown plugin by default whenever you run Jupyter Notebook do the following: First, generate a Jupyter Notebook configuration file (if it has already been generated, you can skip this step).

```
jupyter notebook --generate-config
```

Then, add the following line to the end of the Jupyter Notebook configuration file (for Linux/macOS, usually in the path `~/.jupyter/jupyter_notebook_config.py`):

```
c.NotebookApp.contents_manager_class = 'notedown.NotedownContentsManager'
```

After that, you only need to run the `jupyter notebook` command to turn on the notedown plugin by default.

### Run Jupyter Notebook on a Remote Server

Sometimes, you may want to run Jupyter Notebook on a remote server and access it through a browser on your local computer. If Linux or MacOS is installed on your local machine (Windows can also support this function through third-party software such as PuTTY), you can use port forwarding:

```
ssh myserver -L 8888:localhost:8888
```

The above is the address of the remote server `myserver`. Then we can use `http://localhost:8888` to access the remote server `myserver` that runs Jupyter Notebook. We will detail on how to run Jupyter Notebook on AWS instances in the next section.

### Timing

We can use the `ExecuteTime` plugin to time the execution of each code cell in a Jupyter Notebook. Use the following commands to install the plugin:

```
pip install jupyter_contrib_nbextensions
jupyter contrib nbextension install --user
jupyter nbextension enable execute_time/ExecuteTime
```

### 17.3.3 Summary

- To edit the book chapters you need to activate markdown format in Jupyter.
- You can run servers remotely using port forwarding.

### 17.3.4 Exercises

1. Try to edit and run the code in this book locally.
2. Try to edit and run the code in this book *remotely* via port forwarding.
3. Measure  $\mathbf{A}^\top \mathbf{B}$  vs.  $\mathbf{AB}$  for two square matrices in  $\mathbb{R}^{1024 \times 1024}$ . Which one is faster?

### 17.3.5 Scan the QR Code to Discuss<sup>212</sup>



<sup>212</sup> <https://discuss.mxnet.io/t/2398>

## 17.4 Using AWS Instances

Many deep learning applications require significant amounts of computation. Your local machine might be too slow to solve these problems in a reasonable amount of time. Cloud computing services can give you access to more powerful computers to run the GPU intensive portions of this book. In this section, we will show you how to set up an instance. We will use Jupyter Notebooks to run code on AWS (Amazon Web Services). The walkthrough includes a number of steps:

1. Request for a GPU instance.
2. Optionally: install CUDA or use an AMI with CUDA preinstalled.
3. Set up the corresponding MXNet GPU version.

This process applies to other instances (and other clouds), too, albeit with some minor modifications.

### 17.4.1 Register Account and Log In

First, we need to register an account at <https://aws.amazon.com/>. We strongly encourage you to use two-factor authentication for additional security. Furthermore, it is a good idea to set up detailed billing and spending alerts to avoid any unexpected surprises if you forget to suspend your computers. Note that you will need a credit card. After logging into your AWS account, click “EC2” (marked by the red box in Fig. 17.4.1) to go to the EC2 panel.

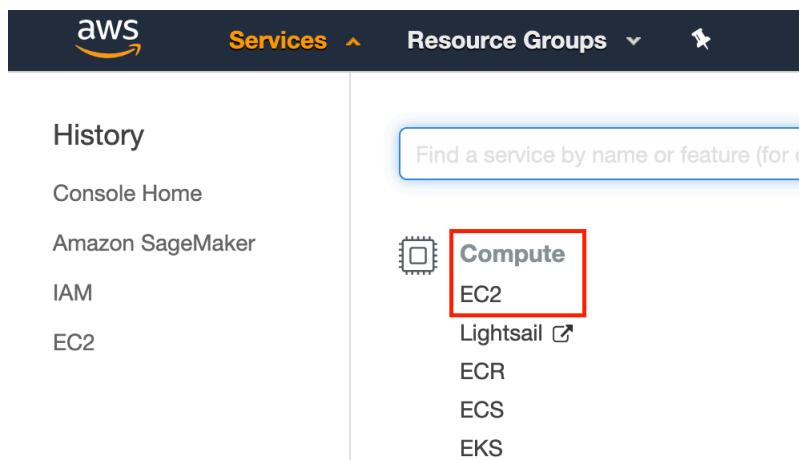


Fig. 17.4.1: Open the EC2 console.

### 17.4.2 Create and Run an EC2 Instance

Fig. 17.4.2 shows the EC2 panel with sensitive account information greyed out. Select a nearby data center to reduce latency, e.g. Oregon. If you are located in China you can select a nearby Asia Pacific region, such as Seoul or Tokyo. Please note that some data centers may not have GPU instances. Click the “Launch Instance” button marked by the red box in Fig. 17.4.2 to launch your instance.

We begin by selecting a suitable AMI (AWS Machine Image). If you want to install everything including the CUDA drivers from scratch, choose Ubuntu. Instead we recommend that you use the Deep Learning AMI that comes with all the drivers preconfigured.

The row at the top of Fig. 17.4.3 shows the steps required to configure the instance. Search for *Deep Learning Base* and select the Ubuntu flavor.

The screenshot shows the AWS EC2 Dashboard. On the left, there's a sidebar with navigation links like 'EC2 Dashboard', 'Instances', 'Images', etc. The main area is titled 'Resources' and shows a list of EC2 resources: Running Instances, Dedicated Hosts, Volumes, Key Pairs, Placement Groups, Elastic IPs, Snapshots, Load Balancers, and Security Groups. Below this, a box contains the text 'Learn more about the latest in AWS Compute from AWS re:Invent by viewing the EC2 Videos.' At the bottom of the main area, there's a 'Create Instance' section with a 'Launch Instance' button, which is also highlighted with a red box.

Fig. 17.4.2: EC2 panel.

This screenshot shows the 'Step 1: Choose an Amazon Machine Image (AMI)' page of the EC2 instance creation wizard. The top navigation bar includes tabs for '1. Choose AMI', '2. Choose Instance Type', '3. Configure Instance', '4. Add Storage', '5. Add Tags', '6. Configure Security Group', and '7. Review'. A search bar at the top has 'deep learning base' typed into it. On the left, a sidebar lists 'Quick Start (3)' options: 'My AMIs (0)', 'AWS Marketplace (9)', 'Community AMIs (44)', and a checked 'Free tier only' checkbox. On the right, a search result for 'Deep Learning Base AMI (Ubuntu) Version 17.0 - ami-0ff00f007c727c376' is shown. This result includes a 'Select' button, a note that it's '64-bit (x86)', and a description: 'Comes with foundational platform of NVidia CUDA, cuDNN, NCCL, GPU Drivers, Intel MKL-DNN and other system libraries to deploy your own custom deep learning environment. For a fully managed experience, check: https://aws.amazon.com/sagemaker'. Below the description are details: 'Root device type: ebs', 'Virtualization type: hvm', and 'ENAv Enabled: Yes'.

Fig. 17.4.3: Choose an operating system.

EC2 provides many different instance configurations to choose from. This can sometimes feel overwhelming to a beginner. Here's a table of suitable machines:

Name	GPU	Notes
g2	Grid K520	ancient
p2	Kepler K80	old but often cheap as spot
g3	Maxwell M60	good trade-off
p3	Volta V100	high performance for FP16
g4	Turing T4	inference optimized FP16/INT8

All the above servers come in multiple flavors indicating the number of GPUs used. E.g. a p2.xlarge has 1 GPU and a p2.16xlarge has 16 GPUs and more memory. For more details see e.g. the [AWS EC2 documentation](#)<sup>213</sup> or a [summary page](#)<sup>214</sup>. For the purpose of illustration a p2.xlarge will suffice.

**Note:** you must use a GPU enabled instance with suitable drivers and a version of MXNet that is GPU enabled. Otherwise you will not see any benefit from using GPUs.

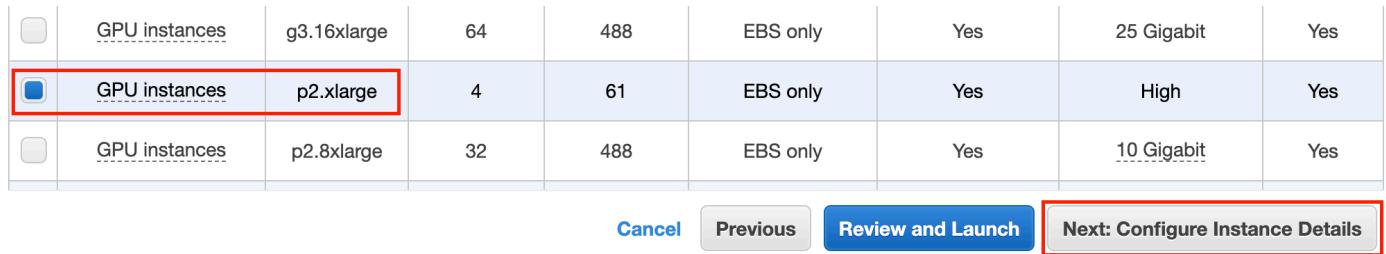


Fig. 17.4.4: Choose an instance.

Before choosing an instance, we suggest you check if there are quantity restrictions by clicking the “Limits” label in the bar on the left as shown in Fig. 17.4.4. Fig. 17.4.5 shows an example of such a limitation. The account can only open one “p2.xlarge” instance per region. If you need to open more instances, click on the “Request limit increase” link to apply for a higher instance quota. Generally, it takes one business day to process an application.

EC2 Dashboard	Running On-Demand p2.16xlarge instances	0	<a href="#">Request limit increase</a>
Events	Running On-Demand p2.8xlarge instances	0	<a href="#">Request limit increase</a>
Tags	Running On-Demand p2.xlarge instances	0	<a href="#">Request limit increase</a>
Reports	Running On-Demand p3.16xlarge instances	0	<a href="#">Request limit increase</a>
Limits			

Fig. 17.4.5: Instance quantity restrictions.

So far, we have finished the first two of seven steps for launching an EC2 instance, as shown on the top of Fig 14.13. In this example, we keep the default configurations for the steps “3. Configure Instance”, “5. Add Tags”, and “6. Configure Security Group”. Tap on “4. Add Storage” and increase the default hard disk size to 64 GB. Note that CUDA by itself already takes up 4GB.

Finally, go to “7. Review” and click “Launch” to launch the configured instance. The system will now prompt you to select the key pair used to access the instance. If you do not have a key pair, select “Create a new key pair” in the first drop-down menu in Fig. 17.4.7 to generate a key pair. Subsequently, you can

<sup>213</sup> <https://aws.amazon.com/ec2/instance-types/>

<sup>214</sup> <https://www.ec2instances.info>

1. Choose AMI    2. Choose Instance Type    3. Configure Instance    4. Add Storage    5. Add Tags    6. Configure Security Group    7. Review

## Step 4: Add Storage

Your instance will be launched with the following storage device settings. You can attach additional EBS volumes and instance store volumes to your instance, or edit the settings of the root volume. You can also attach additional EBS volumes after launching an instance, but not instance store volumes. [Learn more](#) about storage options in Amazon EC2.

Volume Type	Device	Snapshot	Size (GiB)	Volume Type	IOPS	Throughput (MB/s)	Delete on Termination	Encrypted
Root	/dev/sda1	snap-0ba4956ec10715d33	64	General Purpose S	192 / 3000	N/A	<input checked="" type="checkbox"/>	Not Encrypted

Fig. 17.4.6: Modify instance hard disk size.

select “Choose an existing key pair” for this menu and then select the previously generated key pair. Click “Launch Instances” to launch the created instance.

## Select an existing key pair or create a new key pair

A key pair consists of a **public key** that AWS stores, and a **private key file** that you store. Together, they allow you to connect to your instance securely. For Windows AMIs, the private key file is required to obtain the password used to log into your instance. For Linux AMIs, the private key file allows you to securely SSH into your instance.

Note: The selected key pair will be added to the set of keys authorized for this instance. Learn more about [removing existing key pairs from a public AMI](#).

**Create a new key pair**

**Key pair name**

**Download Key Pair**

Fig. 17.4.7: Select a key pair.

Make sure that you download the keypair and store it in a safe location if you generated a new one. This is your only way to SSH into the server. Click the instance ID shown in Fig. 17.4.8 to view the status of this instance.

As shown in Fig. 17.4.9, after the instance state turns green, right-click the instance and select “Connect” to view the instance access method. For example, enter the following in the command line:

```
ssh -i "/path/to/key.pem" ubuntu@ec2-xx-xxx-xxx-xx.y.compute.amazonaws.com
```

Here, “/path/to/key.pem” is the path of the locally-stored key used to access the instance. When the command line prompts “Are you sure you want to continue connecting (yes/no)”, enter “yes” and press Enter to log into the instance.



## Your instances are now launching

The following instance launches have been initiated: i-071ee

[View launch log](#)

Fig. 17.4.8: Click the instance ID.

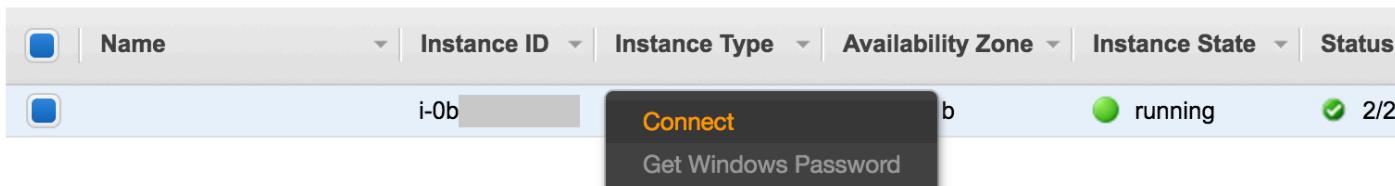


Fig. 17.4.9: View instance access and startup method.

It is a good idea to update the instance with the latest drivers.

```
sudo apt-get update
sudo apt-get dist-upgrade
```

Your server is ready now.

### 17.4.3 Installing CUDA

If you used the Deep Learning AMI you can skip the steps below since it already comes with a range of CUDA versions pre-installed. Instead, all you need to do is select the CUDA version of your choice as follows:

```
sudo rm /usr/local/cuda
sudo ln -s /usr/local/cuda-10.0 /usr/local/cuda
```

This selects CUDA 10.0 as the default.

If you prefer to take the scenic route, please follow the path below. First, update and install the package needed for compilation.

```
sudo apt update
sudo apt dist-upgrade
sudo apt install -y build-essential git libgfortran3
```

NVIDIA frequently releases updates to CUDA (typically one major version per year). Here we download CUDA 10.0. Visit NVIDIA's official repository at (<https://developer.nvidia.com/cuda-toolkit-archive>) to find the download link of CUDA 10.0 as shown below.

After copying the download address in the browser, download and install CUDA 10.0. Presently the following link is up to date:

```
# The download link and file name are subject to change, so always use those
# from the NVIDIA website
wget https://developer.nvidia.com/compute/cuda/10.0/Prod/local_installers/cuda_10.0.130_
↪410.48_linux
sudo sh cuda_10.0.130_410.48_linux
```

Press “Ctrl+C” to jump out of the document and answer the following questions.

**Select Target Platform ⓘ**

Click on the green buttons that describe your target platform. Only supported platforms will be shown.

<b>Operating System</b>	Windows	Linux	Mac OSX			
<b>Architecture ⓘ</b>	x86_64	ppc64le				
<b>Distribution</b>	Fedora	OpenSUSE	RHEL	CentOS	SLES	Ubuntu
<b>Version</b>	18.04	16.04	14.04			
<b>Installer Type ⓘ</b>	runfile (local)	deb (local)	deb (network)	cluster (local)		

Fig. 17.4.10: Find the CUDA 10.0 download address.

```
The NVIDIA CUDA Toolkit provides command-line and graphical
tools for building, debugging and optimizing the performance
Do you accept the previously read EULA?
accept/decline/quit: accept

Install NVIDIA Accelerated Graphics Driver for Linux-x86_64 410.48?
(y)es/(n)o/(q)uit: y

Do you want to install the OpenGL libraries?
(y)es/(n)o/(q)uit [ default is yes ]: y

Do you want to run nvidia-xconfig?
This will update the system X configuration file so that the NVIDIA X driver
is used. The pre-existing X configuration file will be backed up.
This option should not be used on systems that require a custom
X configuration, such as systems with multiple GPU vendors.
(y)es/(n)o/(q)uit [ default is no ]: n

Install the CUDA 10.0 Toolkit?
(y)es/(n)o/(q)uit: y

Enter Toolkit Location
[ default is /usr/local/cuda-10.0 ]:

Do you want to install a symbolic link at /usr/local/cuda?
(y)es/(n)o/(q)uit: y

Install the CUDA 10.0 Samples?
(y)es/(n)o/(q)uit: n
```

After installing the program, run the following command to view the instance GPU.

```
nvidia-smi
```

Finally, add CUDA to the library path to help other libraries find it.

```
echo "export LD_LIBRARY_PATH=\${LD_LIBRARY_PATH}:/usr/local/cuda/lib64" >> ~/.bashrc
```

#### 17.4.4 Install MXNet and Download the D2L Notebooks

For detailed instructions see the introduction where we discussed how to get started with gluon in *Installation* (page 7). First, install Miniconda for Linux.

```
# The download link and file name are subject to change, so always use those
# from the Miniconda website
wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
sudo sh Miniconda3-latest-Linux-x86_64.sh
```

Now, you need to answer the following questions:

```
Do you accept the license terms? [yes|no]
[no] >>> yes
Do you wish the installer to prepend the Miniconda3 install location
to PATH in your /home/ubuntu/.bashrc ? [yes|no]
[no] >>> yes
```

After installation, run `source ~/.bashrc` once to activate CUDA and Conda. Next, download the code for this book and install and activate the Conda environment. To use GPUs you need to update MXNet to request the CUDA 10.0 build.

```
sudo apt-get install unzip
mkdir d2l-en && cd d2l-en
wget https://www.d2l.ai/d2l-en.zip
unzip d2l-en.zip && rm d2l-en.zip
sed -i 's/mxnet/mxnet-cu100/g' environment.yml
conda env create -f environment.yml
source activate gluon
```

You can test quickly whether everything went well as follows:

```
$ conda activate gluon
$ python
>>> import mxnet as mx
>>> ctx = mx.gpu(0)
>>> x = mx.nd.array.zeros(shape=(1024,1024), ctx=ctx)
```

#### 17.4.5 Running Jupyter

To run Jupyter remotely you need to use SSH port forwarding. After all, the server in the cloud doesn't have a monitor or keyboard. For this, log into your server from your desktop (or laptop) as follows.

```
# This command must be run in the local command line
ssh -i "/path/to/key.pem" ubuntu@ec2-xx-xxx-xxx-xx.y.compute.amazonaws.com -L
˓→8889:localhost:8888
conda activate gluon
jupyter notebook
```

Fig. 17.4.11 shows the possible output after you run Jupyter Notebook. The last row is the URL for port 8888.

```
Last login: Sat Apr 20 06:12:12 2019 from 69.181
(base) ubuntu@ip-172-31-2-208:~$ source activate gluon
(gluon) ubuntu@ip-172-31-2-208:~$ jupyter notebook
[I 06:12:41.588 NotebookApp] Writing notebook server cookie secret to /run/user/1000/jupyter/notebook_cookie_secret
[I 06:12:42.617 NotebookApp] Serving notebooks from local directory: /home/ubuntu
[I 06:12:42.618 NotebookApp] The Jupyter Notebook is running at:
[I 06:12:42.618 NotebookApp] http://localhost:8888/?token=3eb5513
[I 06:12:42.618 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
[W 06:12:42.622 NotebookApp] No web browser found: could not locate runnable browser.
[C 06:12:42.622 NotebookApp]

To access the notebook, open this file in a browser:
  file:///run/user/1000/jupyter/nbserver-21907-open.html
Or copy and paste one of these URLs:
  http://localhost:8888/?token=3eb5513
```

Fig. 17.4.11: Output after running Jupyter Notebook. The last row is the URL for port 8888.

Since you used port forwarding to port 8889 you will need to replace the port number and use the secret as given by Jupyter when opening the URL in your local browser.

### 17.4.6 Closing Unused Instances

As cloud services are billed by the time of use, you should close instances that are not being used. Note that there are alternatives: *Stopping* an instance means that you will be able to start it again. This is akin to switching off the power for your regular server. However, stopped instances will still be billed a small amount for the hard disk space retained. *Terminate* deletes all data associated with it. This includes the disk, hence you cannot start it again. Only do this if you know that you won't need it in the future.

If you want to use the instance as a template for many more instances, right-click on the example in Figure 14.16 Fig. 17.4.9 and select “Image” → “Create” to create an image of the instance. Once this is complete, select “Instance State” → “Terminate” to terminate the instance. The next time you want to use this instance, you can follow the steps for creating and running an EC2 instance described in this section to create an instance based on the saved image. The only difference is that, in “1. Choose AMI” shown in Fig. 17.4.3, you must use the “My AMIs” option on the left to select your saved image. The created instance will retain the information stored on the image hard disk. For example, you will not have to reinstall CUDA and other runtime environments.

### 17.4.7 Summary

- Cloud computing services offer a wide variety of GPU servers.
- You can launch and stop instances on demand without having to buy and build your own computer.
- You need to install suitable GPU drivers before you can use them.

### 17.4.8 Exercises

1. The cloud offers convenience, but it does not come cheap. Find out how to launch spot instances<sup>215</sup> to see how to reduce prices.
2. Experiment with different GPU servers. How fast are they?

<sup>215</sup> <https://aws.amazon.com/ec2/spot/>

3. Experiment with multi-GPU servers. How well can you scale things up?

#### 17.4.9 Scan the QR Code to Discuss<sup>216</sup>



## 17.5 GPU Purchase Guide

Deep learning training generally requires large amounts of computation. At present, GPUs are the most cost-effective hardware accelerators for deep learning. In particular, compared with CPUs, GPUs are cheaper and offer higher performance, often by over an order of magnitude. Furthermore, a single server can support multiple GPUs, up to 8 for high end servers. More typical numbers are up to 4 GPUs for an engineering workstation, since heat, cooling and power requirements escalate quickly beyond what an office building can support. For larger deployments, cloud computing, such as Amazon's P3<sup>217</sup> and G4<sup>218</sup> instances are a much more practical solution.

### 17.5.1 Selecting a Server

There is typically no need to purchase high-end CPUs with many threads since much of the computation occurs on the GPUs. That said, due to the Global Interpreter Lock (GIL) in Python, single-thread performance of a CPU can matter in situations where we have 4-8 GPUs. All things equal, this suggests that CPUs with a smaller number of cores but a higher clock frequency might be a more economical choice. An example might be choosing between a 6 core 4GHz and an 8 core 3.5 GHz CPU. Selecting the former is much preferable, even though its aggregate speed is less. An important consideration is that GPUs use lots of power and thus dissipate lots of heat. This requires very good cooling and a large enough chassis to use the GPUs. Follow the guidelines below if possible:

1. **Power Supply.** GPUs use significant amounts of power. Budget with up to 350W per device (check for the *peak demand* of the graphics card rather than typical demand, since efficient code can use lots of energy). If your power supply isn't up to the demand you'll find that your system becomes unstable.
2. **Chassis Size.** GPUs are large and the auxiliary power connectors often need extra space. Also, large chassis are easier to cool.
3. **GPU Cooling.** If you have large numbers of GPUs you might want to invest in water cooling. Also, aim for *reference designs* even if they have fewer fans, since they are thin enough to allow for air intake between the devices. If you buy a multi-fan GPU it might be too thick to get enough air when installing multiple GPUs and you will run into thermal throttling.
4. **PCIe Slots.** Moving data to and from the GPU (and exchanging it between GPUs) requires lots of bandwidth. We recommend PCIe 3.0 slots with 16 lanes. If you mount multiple GPUs, be sure to carefully read the motherboard description to ensure that 16x bandwidth is still available when multiple GPUs are used at the same time and that you're getting PCIe 3.0 as opposed to PCIe 2.0 for

<sup>216</sup> <https://discuss.mxnet.io/t/2399>

<sup>217</sup> <https://aws.amazon.com/ec2/instance-types/p3/>

<sup>218</sup> <https://aws.amazon.com/blogs/aws/in-the-news-ec2-instances-g4-with-nvidia-t4-gpus/>

the additional slots. Some motherboards downgrade to 8x or even 4x bandwidth with multiple GPUs installed. This is partly due to the number of PCIe lanes that the CPU offers.

In short, here are some recommendations for building a deep learning server:

- **Beginner.** Buy a low end GPU with low power consumption (cheap gaming GPUs suitable for deep learning use 150-200W). If you're lucky your current computer will support it.
- **1 GPU.** A low-end CPU with 4 cores will be plenty sufficient and most motherboards suffice. Aim for at least 32GB DRAM and invest into an SSD for local data access. A power supply with 600W should be sufficient. Buy a GPU with lots of fans.
- **2 GPUs.** A low-end CPU with 4-6 cores will suffice. Aim for 64GB DRAM and invest into an SSD. You will need in the order of 1000W for two high-end GPUs. In terms of mainboards, make sure that they have *two* PCIe 3.0 x16 slots. If you can, get a mainboard that has two free spaces (60mm spacing) between the PCIe 3.0 x16 slots for extra air. In this case, buy two GPUs with lots of fans.
- **4 GPUs.** Make sure that you buy a CPU with relatively fast single-thread speed (i.e. high clock frequency). You will probably need a CPU with a larger number of PCIe lanes, such as an AMD Threadripper. You will likely need relatively expensive mainboards to get 4 PCIe 3.0 x16 slots since they probably need a PLX to multiplex the PCIe lanes. Buy GPUs with reference design that are narrow and let air in between the GPUs. You need a 1600-2000W power supply and the outlet in your office might not support that. This server will probably run *loud and hot*. You don't want it under your desk. 128GB of DRAM is recommended. Get an SSD (1-2TB NVMe) for local storage and a bunch of harddisks in RAID configuration to store your data.
- **8 GPUs.** You need to buy a dedicated multi-GPU server chassis with multiple redundant power supplies (e.g. 2+1 for 1600W per power supply). This will require dual socket server CPUs, 256GB ECC DRAM, a fast network card (10GbE recommended), and you will need to check whether the servers support the *physical form factor* of the GPUs. Airflow and wiring placement differ significantly between consumer and server GPUs (e.g. RTX 2080 vs. Tesla V100). This means that you might not be able to install the consumer GPU in a server due to insufficient clearance for the power cable or lack of a suitable wiring harness (as one of the coauthors painfully discovered).

### 17.5.2 Selecting a GPU

At present, AMD and NVIDIA are the two main manufacturers of dedicated GPUs. NVIDIA was the first to enter the deep learning field and provides better support for deep learning frameworks via CUDA. Therefore, most buyers choose NVIDIA GPUs.

NVIDIA provides two types of GPUs, targeting individual users (e.g. via the GTX and RTX series) and enterprise users (via its Tesla series). The two types of GPUs provide comparable compute power. However, the enterprise user GPUs generally use (passive) forced cooling, more memory, and ECC (error correcting) memory. These GPUs are more suitable for data centers and usually cost ten times more than consumer GPUs.

If you are a large company with 100+ servers you should consider the NVIDIA Tesla series or alternatively use GPU servers in the cloud. For a lab or a small to medium company with 10+ servers the NVIDIA RTX series is likely most cost effective. You can buy preconfigured servers with Supermicro or Asus chassis that hold 4-8 GPUs efficiently.

GPU vendors typically release a new generation every 1-2 years, such as the GTX 1000 (Pascal) series released in 2017 and the RTX 2000 (Turing) series released in 2019. Each series offers several different models that provide different performance levels. GPU performance is primarily a combination of the following three parameters:

1. **Compute power.** Generally we look for 32-bit floating-point compute power. 16-bit floating point training (FP16) is also entering the mainstream. If you are only interested in prediction, you can also

use 8-bit integer. The latest generation of Turing GPUs offers 4-bit acceleration. Unfortunately, at present the algorithms to train low-precision networks are not widespread yet.

2. **Memory size.** As your models become larger or the batches used during training grow bigger, you will need more GPU memory. Check for HBM2 (High Bandwidth Memory) vs. GDDR6 (Graphics DDR) memory. HBM2 is faster but much more expensive.
3. **Memory bandwidth.** You can only get the most out of your compute power when you have sufficient memory bandwidth. Look for wide memory buses if using GDDR6.

For most users, it is enough to look at compute power. Note that many GPUs offer different types of acceleration, e.g. NVIDIA's TensorCores accelerate a subset of operators by 5x. Ensure that your libraries support this. The GPU memory should be no less than 4 GB (8GB is much better). Try to avoid using the GPU also for displaying a GUI (use the built-in graphics instead). If you cannot avoid it, add an extra 2GB of RAM for safety.

The figure below compares the 32-bit floating-point compute power and price of the various GTX 900, GTX 1000 and RTX 2000 series models. The prices are the suggested prices found on Wikipedia.



Fig. 17.5.1: Floating-point compute power and price comparison.

We can see a number of things:

1. Within each series, price and performance are roughly proportional. Titan models command a significant premium for the benefit of larger amounts of GPU memory. However, the newer models offer better cost effectiveness, as can be seen by comparing the 980 Ti and 1080 Ti. The price does not appear to improve much for the RTX 2000 series. However, this is due to the fact that they offer far superior low precision performance (FP16, INT8 and INT4).
2. The performance to cost ratio of the GTX 1000 series is about two times greater than the 900 series.
3. For the RTX 2000 series the price is an *affine* function of the price.



Fig. 17.5.2: Floating-point compute power and energy consumption.

The second curve shows how energy consumption scales mostly linearly with the amount of computation. Secondly, later generations are more efficient. This seems to be contradicted by the graph corresponding to the RTX 2000 series. However, this is a consequence of the TensorCores which draw a disproportional amount of energy.

### 17.5.3 Summary

- Watch out for power, PCIe bus lanes, CPU single thread speed and cooling when building a server.
- You should purchase the latest GPU generation if possible.
- Use the cloud for large deployments.
- High density servers may not be compatible with all GPUs. Check the mechanical and cooling specifications before you buy.
- Use FP16 or lower precision for high efficiency.

### 17.5.4 Scan the QR Code to Discuss<sup>219</sup>

<sup>219</sup> <https://discuss.mxnet.io/t/2400>



## 17.6 How to Contribute to This Book

Contributions by readers<sup>220</sup> help us improve this book. If you find a typo, an outdated link, something where you think we missed a citation, where the code doesn't look elegant or where an explanation is unclear, please contribute back and help us help our readers. While in regular books the delay between print runs (and thus between typo corrections) can be measured in years, it typically takes hours to days to incorporate an improvement in this book. This is all possible due to version control and continuous integration testing. To do so you need to install Git and submit a [pull request<sup>221</sup>](#) to the GitHub repository. When your pull request is merged into the code repository by the author, you will become a contributor. In a nutshell the process works as described in the diagram below.

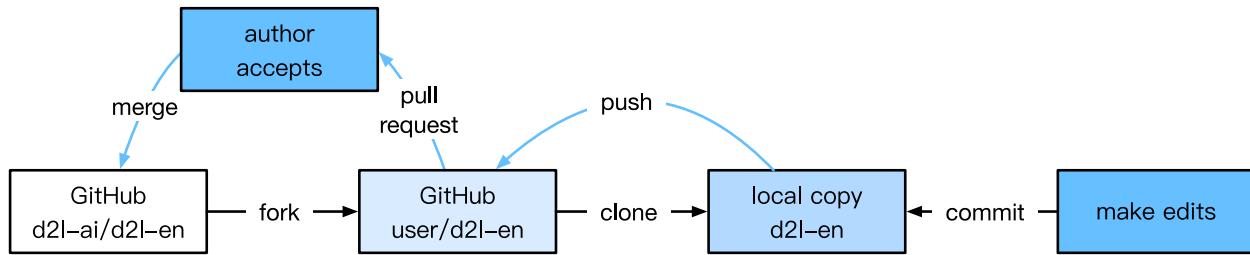


Fig. 17.6.1: Contributing to the book.

### 17.6.1 From Reader to Contributor in 6 Steps

We will walk you through the steps in detail. If you are already familiar with Git you can skip this section. For concreteness we assume that the contributor's user name is `smolix`.

#### Install Git

The Git open source book describes [how to install Git<sup>222</sup>](#). This typically works via `apt install git` on Ubuntu Linux, by installing the Xcode developer tools on macOS, or by using GitHub's desktop client<sup>223</sup>. If you don't have a GitHub account, you need to sign up for one [4].

#### Log in to GitHub

Enter the [address<sup>224</sup>](#) of the book's code repository in your browser. Click on the **Fork** button in the red box at the top-right of the figure below, to make a copy of the repository of this book. This is now *your copy* and you can change it any way you want.

<sup>220</sup> <https://github.com/d2l-ai/d2l-en/graphs/contributors>

<sup>221</sup> <https://github.com/d2l-ai/d2l-en/pulls>

<sup>222</sup> <https://git-scm.com/book/zh/v2>

<sup>223</sup> <https://desktop.github.com>

<sup>224</sup> <https://github.com/d2l-ai/d2l-en/>

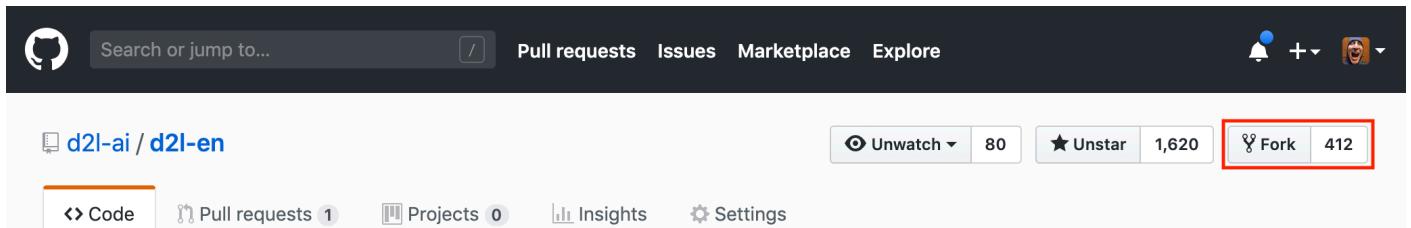


Fig. 17.6.2: The code repository page.

Now, the code repository of this book will be copied to your username, such as `smolix/d2l-en` shown at the top-left of the screenshot below.

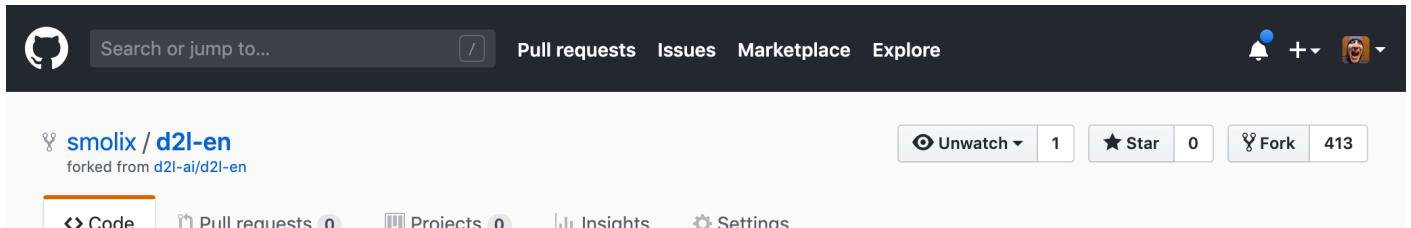


Fig. 17.6.3: Copy the code repository.

## Clone the Repository

To clone the repository (i.e. to make a local copy) we need to get its repository address. The green button on the picture below displays this. Make sure that your local copy is up to date with the main repository if you decide to keep this fork around for longer. For now simply follow the instructions in [Section 2](#) to get started. The main difference is that you're now downloading *your own fork* of the repository.



Fig. 17.6.4: Git clone.

```
# Replace your_github_username with your GitHub username
git clone https://github.com/your_github_username/d2l-en.git
```

On Unix the above command copies all the code from GitHub to the directory `d2l-en`.

## Edit the Book and Push

Now it's time to edit the book. It's best to edit the notebooks in Jupyter following instructions in [Section 17.3](#). Make the changes and check that they're OK. Assume we have modified a typo in the file `~/d2l-en/chapter_appendix/how-to-contribute.md`. You can then check which files you have changed:

```
git status
```

At this point Git will prompt that the `chapter_appendix/how-to-contribute.md` file has been modified.

```
mylaptop:d2l-en smola$ git status
On branch master
Your branch is up-to-date with 'origin/master'.

Changes not staged for commit:
  (use "git add <file>..." to update what will be committed)
  (use "git checkout -- <file>..." to discard changes in working directory)

    modified:   chapter_appendix/how-to-contribute.md
```

After confirming that this is what you want, execute the following command:

```
git add chapter_appendix/how-to-contribute.md
git commit -m 'fix typo in git documentation'
git push
```

The changed code will then be in your personal fork of the repository. To request the addition of your change, you have to create a pull request for the official repository of the book.

## Pull Request

Go to your fork of the repository on GitHub and select “New pull request”. This will open up a screen that shows you the changes between your edits and what is current in the main repository of the book.



Fig. 17.6.5: Pull Request.

## Submit Pull Request

Finally, submit a pull request. Make sure to describe the changes you have made in the pull request. This will make it easier for the authors to review it and to merge it with the book. Depending on the changes, this might get accepted right away, rejected, or more likely, you’ll get some feedback on the changes. Once you’ve incorporated them, you’re good to go.

Your pull request will appear among the list of requests in the main repository. We will make every effort to process it quickly.

### 17.6.2 Summary

- You can use GitHub to contribute to this book.

## Comparing changes

Choose two branches to see what's changed or to start a new pull request. If you need to, you can also [compare across forks](#).

base repository: d2l-ai/d2l-en ▾ base: master ↲ head repository: smolix/d2l-en ▾ compare: master ▾

✓ Able to merge. These branches can be automatically merged.

**Create pull request** Discuss and review the changes in this comparison with others. ?

• 1 commit 1 file changed 0 commit comments 1 contributor

Fig. 17.6.6: Create Pull Request.

- Forking a repository is the first step to contributing, since it allows you to edit things locally and only contribute back once you're ready.
- Pull requests are how contributions are being bundled up. Try not to submit huge pull requests since this makes them hard to understand and incorporate. Better send several smaller ones.

### 17.6.3 Exercises

1. Star and fork the `d2l-en` repository.
2. Find some code that needs improvement and submit a pull request.
3. Find a reference that we missed and submit a pull request.

### 17.6.4 Scan the QR Code to Discuss<sup>225</sup>



## 17.7 d2l API Document

```
class d2l.Accumulator(n)
    Sum a list of numbers over time

class d2l.Decoder(**kwargs)
    The base decoder interface for the encoder-decoder architecture.

    forward(X, state)
        Overrides to implement forward computation using NDArray. Only accepts positional arguments.
        *args [list of NDArray] Input tensors.
```

<sup>225</sup> <https://discuss.mxnet.io/t/2401>

```
class d2l.DotProductAttention(dropout, **kwargs)

    forward(query, key, value, valid_length=None)
        Overrides to implement forward computation using NDArray. Only accepts positional arguments.
        *args [list of NDArray] Input tensors.

class d2l.Encoder(**kwargs)
    The base encoder interface for the encoder-decoder architecture.

    forward(X)
        Overrides to implement forward computation using NDArray. Only accepts positional arguments.
        *args [list of NDArray] Input tensors.

class d2l.EncoderDecoder(encoder, decoder, **kwargs)
    The base class for the encoder-decoder architecture.

    forward(enc_X, dec_X, *args)
        Overrides to implement forward computation using NDArray. Only accepts positional arguments.
        *args [list of NDArray] Input tensors.

class d2l.MLPAttention(units, dropout, **kwargs)

    forward(query, key, value, valid_length)
        Overrides to implement forward computation using NDArray. Only accepts positional arguments.
        *args [list of NDArray] Input tensors.

class d2l.MaskedSoftmaxCELoss(axis=-1, sparse_label=True, from_logits=False, weight=None,
                                batch_axis=0, **kwargs)

    forward(pred, label, valid_length)
        Defines the forward computation. Arguments can be either NDArray or Symbol.

class d2l.RNNModel(rnn_layer, vocab_size, **kwargs)

    forward(inputs, state)
        Overrides to implement forward computation using NDArray. Only accepts positional arguments.
        *args [list of NDArray] Input tensors.

class d2l.RNNModelScratch(vocab_size, num_hiddens, ctx, get_params, init_state, forward)
    A RNN Model based on scratch implementations

class d2l.RandomGenerator(sampling_weights)
    Draw a random int in [0, n] according to n sampling weights

class d2l.Residual(num_channels, use_1x1conv=False, strides=1, **kwargs)

    forward(X)
        Overrides to implement forward computation using NDArray. Only accepts positional arguments.
        *args [list of NDArray] Input tensors.

class d2l.Seq2SeqDecoder(vocab_size, embed_size, num_hiddens, num_layers, dropout=0,
                         **kwargs)

    forward(X, state)
        Overrides to implement forward computation using NDArray. Only accepts positional arguments.
```

```

*args [list of NDArray] Input tensors.

class d2l.Seq2SeqEncoder(vocab_size, embed_size, num_hiddens, num_layers, dropout=0,
    **kwargs

forward(X, *args)
    Overrides to implement forward computation using NDArray. Only accepts positional arguments.

*args [list of NDArray] Input tensors.

class d2l.SeqDataLoader(batch_size, num_steps, use_random_iter, max_tokens)
    A iterator to load sequence data

class d2l.Timer
    Record multiple running times.

avg()
    Return the average time

cumsum()
    Return the accumulated times

start()
    Start the timer

stop()
    Stop the timer and record the time in a list

sum()
    Return the sum of time

class d2l.VOCSegDataset(is_train, crop_size, voc_dir)
    A customized dataset to load VOC dataset.

d2l.bbox_to_rect(bbox, color)
    Convert bounding box to matplotlib format.

d2l.build_colormap2label()
    Build a RGB color to label mapping for segmentation.

d2l.corr2d(X, K)
    Compute 2D cross-correlation.

d2l.download_voc_pascal(data_dir='./data')
    Download the VOC2012 segmentation dataset.

d2l.evaluate_loss(net, data_iter, loss)
    Evaluate the loss of a model on the given dataset

d2l.load_array(data_arrays, batch_size, is_train=True)
    Construct a Gluon data loader

d2l.load_data_fashion_mnist(batch_size, resize=None)
    Download the Fashion-MNIST dataset and then load into memory.

d2l.load_data_pikachu(batch_size, edge_size=256)
    Load the pikachu dataset

d2l.load_data_voc(batch_size, crop_size)
    Download and load the VOC2012 semantic dataset.

d2l.plot(X, Y=None, xlabel=None, ylabel=None, legend=[], xlim=None, ylim=None, xscale='linear',
    yscale='linear', fmts=None, figsize=(3.5, 2.5), axes=None)
    Plot multiple lines

```

```
d2l.read_time_machine()
    Load the time machine book into a list of sentences.

d2l.read_voc_images(root='./data/VOCdevkit/VOC2012', is_train=True)
    Read all VOC feature and label images.

d2l.resnet18(num_classes)
    A slightly modified ResNet-18 model

d2l.set_axes(axes, xlabel, ylabel, xlim, ylim, xscale, yscale, legend)
    A utility function to set matplotlib axes

d2l.set_figsize(figsize=(3.5, 2.5))
    Change the default figure size

d2l.show_bboxes(axes, bboxes, labels=None, colors=None)
    Show bounding boxes.

d2l.show_images(imgs, num_rows, num_cols, titles=None, scale=1.5)
    Plot a list of images.

d2l.show_trace_2d(f, results)
    Show the trace of 2D variables during optimization.

d2l.split_batch(X, y, ctx_list)
    Split X and y into multiple devices specified by ctx

d2l.synthetic_data(w, b, num_examples)
    generate y = X w + b + noise

d2l.tokenize(lines, token='word')
    Split sentences into word or char tokens

d2l.train_2d(trainer)
    Optimize a 2-dim objective function with a customized trainer.

d2l.try_all_gpus()
    Return all available GPUs, or [cpu(),] if no GPU exists.

d2l.try_gpu(i=0)
    Return gpu(i) if exists, otherwise return cpu().

d2l.update_D(X, Z, net_D, net_G, loss, trainer_D)
    Update discriminator

d2l.update_G(Z, net_D, net_G, loss, trainer_G)
    Update generator

d2l.use_svg_display()
    Use the svg format to display plot in jupyter.

d2l.voc_label_indices(colormap, colormap2label)
    Map a RGB color to a label.

d2l.voc_rand_crop(feature, label, height, width)
    Randomly crop for both feature and label images.
```

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