6.036 Lecture Notes

Contents

CHAPTER 1

Introduction

The main focus of machine learning is *making decisions or predictions based on data*. There are a number of other fields with significant overlap in technique, but difference in focus: in economics and psychology, the goal is to discover underlying causal processes and in statistics it is to find a model that fits a data set well. In those fields, the end product is a model. In machine learning, we often fit models, but as a means to the end of making good predictions or decisions.

This story paraphrased from a post on 9/4/12 at andrewgelman.com

As machine-learning (ML) methods have improved in their capability and scope, ML has become the best way, measured in terms of speed, human engineering time, and robustness, to make many applications. Great examples are face detection and speech recognition and many kinds of language-processing tasks. Almost any application that involves understanding data or signals that come from the real world can be best addressed using machine learning.

One crucial aspect of machine learning approaches to solving problems is that human engineering plays an important role. A human still has to *frame* the problem: acquire and organize data, design a space of possible solutions, select a learning algorithm and its parameters, apply the algorithm to the data, validate the resulting solution to decide whether it's good enough to use, etc. These steps are of great importance.

and often undervalued

The conceptual basis of learning from data is the *problem of induction*: Why do we think that previously seen data will help us predict the future? This is a serious philosophical problem of long standing. We will operationalize it by making assumptions, such as that all training data are IID (independent and identically distributed) and that queries will be drawn from the same distribution as the training data, or that the answer comes from a set of possible answers known in advance.

In general, we need to solve these two problems:

- **estimation:** When we have data that are noisy reflections of some underlying quantity of interest, we have to aggregate the data and make estimates or predictions about the quantity. How do we deal with the fact that, for example, the same treatment may end up with different results on different trials? How can we predict how well an estimate may compare to future results?
- **generalization:** How can we predict results of a situation or experiment that we have never encountered before in our data set?

We can describe problems and their solutions using six characteristics, three of which characterize the problem and three of which characterize the solution:

1. **Problem class:** What is the nature of the training data and what kinds of queries will be made at testing time?
2. **Assumptions:** What do we know about the source of the data or the form of the solution?
3. **Evaluation criteria:** What is the goal of the prediction or estimation system? How will the answers to individual queries be evaluated? How will the overall performance of the system be measured?
4. **Model type:** Will an intermediate model be made? What aspects of the data will be modeled? How will the model be used to make predictions?
5. **Model class:** What particular parametric class of models will be used? What criterion will we use to pick a particular model from the model class?
6. **Algorithm:** What computational process will be used to fit the model to the data and/or to make predictions?

Without making some assumptions about the nature of the process generating the data, we cannot perform generalization. In the following sections, we elaborate on these ideas.

Don't feel you have to memorize all these kinds of learning, etc. We just want you to have a very high-level view of (part of) the breadth of the field.

1 Problem class

There are many different *problem classes* in machine learning. They vary according to what kind of data is provided and what kind of conclusions are to be drawn from it. Five standard problem classes are described below, to establish some notation and terminology.

In this course, we will focus on classification and regression (two examples of supervised learning), and will touch on reinforcement learning and sequence learning.

1.1 Supervised learning

The idea of *supervised* learning is that the learning system is given inputs and told which specific outputs should be associated with them. We divide up supervised learning based on whether the outputs are drawn from a small finite set (classification) or a large finite or continuous set (regression).

1.1.1 Classification

Training data $\mathcal{D}_n$ is in the form of a set of pairs $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$ where $x^{(i)}$ represents an object to be classified, most typically a d-dimensional vector of real and/or discrete values, and $y^{(i)}$ is an element of a discrete set of values. The y values are sometimes called *target values*.

A classification problem is *binary* or *two-class* if $y^{(i)}$ is drawn from a set of two possible values; otherwise, it is called *multi-class*.

The goal in a classification problem is ultimately, given a new input value $x^{(n+1)}$, to predict the value of $y^{(n+1)}$.

Classification problems are a kind of *supervised learning*, because the desired output (or class) $y^{(i)}$ is specified for each of the training examples $x^{(i)}$.

Many textbooks use x_i and t_i instead of $x^{(i)}$ and $y^{(i)}$. We find that notation somewhat difficult to manage when $x^{(i)}$ is itself a vector and we need to talk about its elements. The notation we are using is standard in some other parts of the machine-learning literature.

1.1.2 Regression

Regression is like classification, except that $y^{(i)} \in \mathbb{R}^k$.

1.2 Unsupervised learning

Unsupervised learning doesn't involve learning a function from inputs to outputs based on a set of input-output pairs. Instead, one is given a data set and generally expected to find some patterns or structure inherent in it.

1.2.1 Density estimation

Given samples $x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}^d$ drawn IID from some distribution $\Pr(X)$, the goal is to predict the probability $\Pr(x^{(n+1)})$ of an element drawn from the same distribution. Density estimation sometimes plays a role as a "subroutine" in the overall learning method for supervised learning, as well.

IID stands for *independent and identically distributed*, which means that the elements in the set are related in the sense that they all come from the same underlying probability distribution, but not in any other ways.

1.2.2 Clustering

Given samples $x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}^d$, the goal is to find a partitioning (or "clustering") of the samples that groups together samples that are similar. There are many different objectives, depending on the definition of the similarity between samples and exactly what criterion is to be used (e.g., minimize the average distance between elements inside a cluster and maximize the average distance between elements across clusters). Other methods perform a "soft" clustering, in which samples may be assigned 0.9 membership in one cluster and 0.1 in another. Clustering is sometimes used as a step in density estimation, and sometimes to find useful structure in data.

1.2.3 Dimensionality reduction

Given samples $x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}^D$, the problem is to re-represent them as points in a d-dimensional space, where $d < D$. The goal is typically to retain information in the data set that will, e.g., allow elements of one class to be discriminated from another.

Dimensionality reduction is a standard technique which is particularly useful for visualizing or understanding high-dimensional data. If the goal is ultimately to perform regression or classification on the data after the dimensionality is reduced, it is usually best to articulate an objective for the overall prediction problem rather than to first do dimensionality reduction without knowing which dimensions will be important for the prediction task.

1.3 Reinforcement learning

In reinforcement learning, the goal is to learn a mapping from input values x to output values y, but without a direct supervision signal to specify which output values y are best for a particular input. There is no training set specified *a priori*. Instead, the learning problem is framed as an agent interacting with an environment, in the following setting:

- The agent observes the current state, $x^{(0)}$.
- It selects an action, $y^{(0)}$.
- It receives a reward, $r^{(0)}$, which depends on $x^{(0)}$ and possibly $y^{(0)}$.
- The environment transitions probabilistically to a new state, $x^{(1)}$, with a distribution that depends only on $x^{(0)}$ and $y^{(0)}$.

- The agent observes the current state, $x^{(1)}$.
- ...

The goal is to find a policy π, mapping x to y, (that is, states to actions) such that some long-term sum or average of rewards r is maximized.

This setting is very different from either supervised learning or unsupervised learning, because the agent's action choices affect both its reward and its ability to observe the environment. It requires careful consideration of the long-term effects of actions, as well as all of the other issues that pertain to supervised learning.

1.4 Sequence learning

In sequence learning, the goal is to learn a mapping from *input sequences* $x_0, \ldots, x_n$ to *output sequences* $y_1, \ldots, y_m$. The mapping is typically represented as a *state machine*, with one function f used to compute the next hidden internal state given the input, and another function g used to compute the output given the current hidden state.

It is supervised in the sense that we are told what output sequence to generate for which input sequence, but the internal functions have to be learned by some method other than direct supervision, because we don't know what the hidden state sequence is.

1.5 Other settings

There are many other problem settings. Here are a few.

In *semi-supervised* learning, we have a supervised-learning training set, but there may be an additional set of $x^{(i)}$ values with no known $y^{(i)}$. These values can still be used to improve learning performance if they are drawn from $\Pr(X)$ that is the marginal of $\Pr(X, Y)$ that governs the rest of the data set.

In *active* learning, it is assumed to be expensive to acquire a label $y^{(i)}$ (imagine asking a human to read an x-ray image), so the learning algorithm can sequentially ask for particular inputs $x^{(i)}$ to be labeled, and must carefully select queries in order to learn as effectively as possible while minimizing the cost of labeling.

In *transfer* learning (also called *meta-learning*), there are multiple tasks, with data drawn from different, but related, distributions. The goal is for experience with previous tasks to apply to learning a current task in a way that requires decreased experience with the new task.

2 Assumptions

The kinds of assumptions that we can make about the data source or the solution include:

- The data are independent and identically distributed.
- The data are generated by a Markov chain.
- The process generating the data might be adversarial.
- The "true" model that is generating the data can be perfectly described by one of some particular set of hypotheses.

The effect of an assumption is often to reduce the "size" or "expressiveness" of the space of possible hypotheses and therefore reduce the amount of data required to reliably identify an appropriate hypothesis.

3 Evaluation criteria

Once we have specified a problem class, we need to say what makes an output or the answer to a query good, given the training data. We specify evaluation criteria at two levels: how an individual prediction is scored, and how the overall behavior of the prediction or estimation system is scored.

The quality of predictions from a learned model is often expressed in terms of a *loss function*. A loss function $L(g, a)$ tells you how much you will be penalized for making a guess g when the answer is actually a. There are many possible loss functions. Here are some frequently used examples:

- **0-1 Loss** applies to predictions drawn from finite domains.

$$L(g, a) = \begin{cases} 0 & \text{if } g = a \\ 1 & \text{otherwise} \end{cases}$$

If the actual values are drawn from a continuous distribution, the probability they would ever be equal to some predicted g is 0 (except for some weird cases).

- **Squared loss**

$$L(g, a) = (g - a)^2$$

- **Linear loss**

$$L(g, a) = |g - a|$$

- **Asymmetric loss** Consider a situation in which you are trying to predict whether someone is having a heart attack. It might be much worse to predict "no" when the answer is really "yes", than the other way around.

$$L(g, a) = \begin{cases} 1 & \text{if } g = 1 \text{ and } a = 0 \\ 10 & \text{if } g = 0 \text{ and } a = 1 \\ 0 & \text{otherwise} \end{cases}$$

Any given prediction rule will usually be evaluated based on multiple predictions and the loss of each one. At this level, we might be interested in:

- Minimizing expected loss over all the predictions (also known as risk)
- Minimizing maximum loss: the loss of the worst prediction
- Minimizing or bounding regret: how much worse this predictor performs than the best one drawn from some class
- Characterizing asymptotic behavior: how well the predictor will perform in the limit of infinite training data
- Finding algorithms that are probably approximately correct: they probably generate a hypothesis that is right most of the time.

There is a theory of rational agency that argues that you should always select the action that *minimizes the expected loss*. This strategy will, for example, make you the most money in the long run, in a gambling setting. Expected loss is also sometimes called *risk* in the machine-learning literature, but that term means other things in economics or other parts of decision theory, so be careful...it's risky to use it. We will, most of the time, concentrate on this criterion.

Of course, there are other models for action selection and it's clear that people do not always (or maybe even often) select actions that follow this rule.

4 Model type

Recall that the goal of a machine-learning system is typically to estimate or generalize, based on data provided. Below, we examine the role of model-making in machine learning.

4.1 No model

In some simple cases, in response to queries, we can generate predictions directly from the training data, without the construction of any intermediate model. For example, in regression or classification, we might generate an answer to a new query by averaging answers to recent queries, as in the *nearest neighbor* method.

4.2 Prediction rule

This two-step process is more typical:

1. "Fit" a model to the training data
2. Use the model directly to make predictions

In the *prediction rule* setting of regression or classification, the model will be some hypothesis or prediction rule $y = h(x;\theta)$ for some functional form h. The idea is that θ is a vector of one or more parameter values that will be determined by fitting the model to the training data and then be held fixed. Given a new $x^{(n+1)}$, we would then make the prediction $h(x^{(n+1)};\theta)$.

The fitting process is often articulated as an optimization problem: Find a value of θ that minimizes some criterion involving θ and the data. An optimal strategy, if we knew the actual underlying distribution on our data, $\Pr(X, Y)$ would be to predict the value of y that minimizes the *expected loss*, which is also known as the *test error*. If we don't have that actual underlying distribution, or even an estimate of it, we can take the approach of minimizing the *training error*: that is, finding the prediction rule h that minimizes the average loss on our training data set. So, we would seek θ that minimizes

$$\mathcal{E}_n(\theta) = \frac{1}{n}\sum_{i=1}^{n} L(h(x^{(i)};\theta), y^{(i)}) \ ,$$

where the loss function $L(g, a)$ measures how bad it would be to make a guess of g when the actual value is a.

We will find that minimizing training error alone is often not a good choice: it is possible to emphasize fitting the current data too strongly and end up with a hypothesis that does not generalize well when presented with new x values.

We write $f(a;b)$ to describe a function that is usually applied to a single argument a, but is a member of a parametric family of functions, with the particular function determined by parameter value b. So, for example, we might write $h(x;p) = x^p$ to describe a function of a single argument that is parameterized by p.

5 Model class and parameter fitting

A model *class* $\mathcal{M}$ is a set of possible models, typically parameterized by a vector of parameters Θ. What assumptions will we make about the form of the model? When solving a regression problem using a prediction-rule approach, we might try to find a linear function $h(x;\theta,\theta_0) = \theta^T x + \theta_0$ that fits our data well. In this example, the parameter vector $\Theta = (\theta, \theta_0)$.

For problem types such as discrimination and classification, there are huge numbers of model classes that have been considered...we'll spend much of this course exploring these model classes, especially neural networks models. We will almost completely restrict our

attention to model classes with a fixed, finite number of parameters. Models that relax this assumption are called "non-parametric" models.

How do we select a model class? In some cases, the machine-learning practitioner will have a good idea of what an appropriate model class is, and will specify it directly. In other cases, we may consider several model classes. In such situations, we are solving a *model selection* problem: model-selection is to pick a model class $\mathcal{M}$ from a (usually finite) set of possible model classes; *model fitting* is to pick a particular model in that class, specified by parameters θ.

6 Algorithm

Once we have described a class of models and a way of scoring a model given data, we have an algorithmic problem: what sequence of computational instructions should we run in order to find a good model from our class? For example, determining the parameter vector θ which minimizes $\mathcal{E}_n(\theta)$ might be done using a familiar least-squares minimization algorithm, when the model h is a function being fit to some data x.

Sometimes we can use software that was designed, generically, to perform optimization. In many other cases, we use algorithms that are specialized for machine-learning problems, or for particular hypotheses classes.

Some algorithms are not easily seen as trying to optimize a particular criterion. In fact, the first algorithm we study for finding linear classifiers, the perceptron algorithm, has this character.

CHAPTER 2

Linear classifiers

1 Classification

A binary *classifier* is a mapping from $\mathbb{R}^d \to \{-1, +1\}$. We'll often use the letter h (for hypothesis) to stand for a classifier, so the classification process looks like:

$$x \to \boxed{h} \to y \quad .$$

Actually, general classifiers can have a range which is any discrete set, but we'll work with this specific case for a while.

Real life rarely gives us vectors of real numbers; the x we really want to classify is usually something like a song, image, or person. In that case, we'll have to define a function $\varphi(x)$, whose domain is $\mathbb{R}^d$, where φ represents *features* of x, like a person's height or the amount of bass in a song, and then let the $h : \varphi(x) \to \{-1, +1\}$. In much of the following, we'll omit explicit mention of φ and assume that the $x^{(i)}$ are in $\mathbb{R}^d$, but you should always have in mind that some additional process was almost surely required to go from the actual input examples to their feature representation.

In *supervised learning* we are given a training data set of the form

$$\mathcal{D}_n = \left\{ \left(x^{(1)}, y^{(1)} \right), \ldots, \left(x^{(n)}, y^{(n)} \right) \right\} \quad .$$

We will assume that each $x^{(i)}$ is a $d \times 1$ *column vector*. The intended meaning of this data is that, when given an input $x^{(i)}$, the learned hypothesis should generate output $y^{(i)}$.

What makes a classifier useful? That it works well on *new* data; that is, that it makes good predictions on examples it hasn't seen. But we don't know exactly what data this classifier might be tested on when we use it in the real world. So, we have to *assume* a connection between the training data and testing data; typically, they are drawn independently from the same probability distribution.

My favorite analogy is to problem sets. We evaluate a student's ability to *generalize* by putting questions on the exam that were not on the homework (training set).

Given a training set $\mathcal{D}_n$ and a classifier h, we can define the *training error* of h to be

$$\mathcal{E}_n(h) = \frac{1}{n} \sum_{i=1}^{n} \begin{cases} 1 & h(x^{(i)}) \neq y^{(i)} \\ 0 & \text{otherwise} \end{cases} \quad .$$

For now, we will try to find a classifier with small training error (later, with some added criteria) and hope it *generalizes well* to new data, and has a small *test error*

$$\mathcal{E}(h) = \frac{1}{n'} \sum_{i=n+1}^{n+n'} \begin{cases} 1 & h(x^{(i)}) \neq y^{(i)} \\ 0 & \text{otherwise} \end{cases}$$

on n' new examples that were not used in the process of finding the classifier.

2 Learning algorithm

A *hypothesis class* $\mathcal{H}$ is a set (finite or infinite) of possible classifiers, each of which represents a mapping from $\mathbb{R}^d \to \{-1, +1\}$.

A *learning algorithm* is a procedure that takes a data set $\mathcal{D}_n$ as input and returns an element h of $\mathcal{H}$; it looks like

$$\mathcal{D}_n \longrightarrow \boxed{\text{learning alg } (\mathcal{H})} \longrightarrow h$$

We will find that the choice of $\mathcal{H}$ can have a big impact on the test error of the h that results from this process. One way to get h that generalizes well is to restrict the size, or "expressiveness" of $\mathcal{H}$.

3 Linear classifiers

We'll start with the hypothesis class of *linear classifiers*. They are (relatively) easy to understand, simple in a mathematical sense, powerful on their own, and the basis for many other more sophisticated methods.

A linear classifier in d dimensions is defined by a vector of parameters $\theta \in \mathbb{R}^d$ and scalar $\theta_0 \in \mathbb{R}$. So, the hypothesis class $\mathcal{H}$ of linear classifiers in d dimensions is the *set* of all vectors in $\mathbb{R}^{d+1}$. We'll assume that θ is a $d \times 1$ column vector.

Given particular values for θ and θ_0, the classifier is defined by

$$h(x; \theta, \theta_0) = \text{sign}(\theta^T x + \theta_0) = \begin{cases} +1 & \text{if } \theta^T x + \theta_0 > 0 \\ -1 & \text{otherwise} \end{cases} .$$

Let's be careful about dimensions. We have assumed that x and θ are both $d \times 1$ column vectors. So $\theta^T x$ is 1×1, which in math (but not necessarily numpy) is the same as a scalar.

Remember that we can think of θ, θ_0 as specifying a hyperplane. It divides $\mathbb{R}^d$, the space our $x^{(i)}$ points live in, into two half-spaces. The one that is on the same side as the normal vector is the *positive* half-space, and we classify all points in that space as positive. The half-space on the other side is *negative* and all points in it are classified as negative.

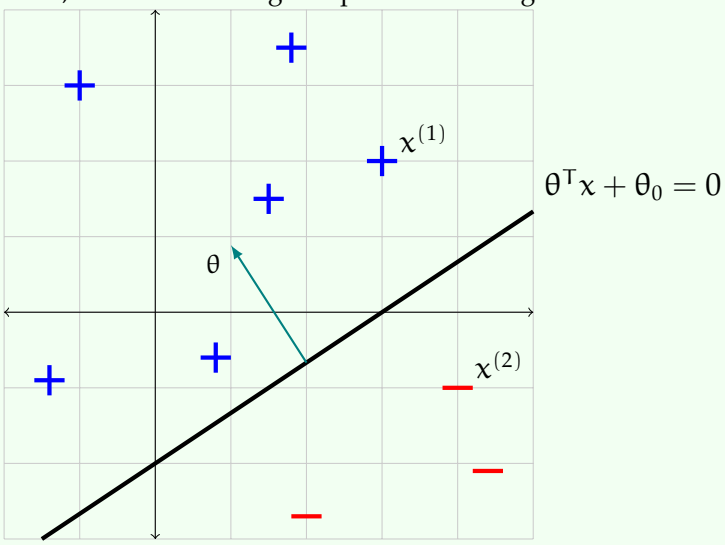
Example: Let h be the linear classifier defined by $\theta = \begin{bmatrix} -1 \\ 1.5 \end{bmatrix}, \theta_0 = 3$.

The diagram below shows several points classified by h. In particular, let $x^{(1)} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$ and $x^{(2)} = \begin{bmatrix} 4 \\ -1 \end{bmatrix}$.

$$h(x^{(1)}; \theta, \theta_0) = \text{sign}\left(\begin{bmatrix} -1 & 1.5 \end{bmatrix} \begin{bmatrix} 3 \\ 2 \end{bmatrix} + 3 \right) = \text{sign}(3) = +1$$

$$h(x^{(2)}; \theta, \theta_0) = \text{sign}\left(\begin{bmatrix} -1 & 1.5 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \end{bmatrix} + 3 \right) = \text{sign}(-2.5) = -1$$

Thus, $x^{(1)}$ and $x^{(2)}$ are given positive and negative classfications, respectively.



Study Question: What is the green vector normal to the hyperplane? Specify it as a column vector.

Study Question: What change would you have to make to θ, θ_0 if you wanted to have the separating hyperplane in the same place, but to classify all the points labeled '+' in the diagram as negative and all the points labeled '-' in the diagram as positive?

4 Learning linear classifiers

Now, given a data set and the hypothesis class of linear classifiers, our objective will be to find the linear classifier with the smallest possible training error.

This is a well-formed optimization problem. But it's not computationally easy!

We'll start by considering a very simple learning algorithm. The idea is to generate k possible hypotheses by generating their parameter vectors at random. Then, we can evaluate the training-set error on each of the hypotheses and return the hypothesis that has the lowest training error (breaking ties arbitrarily).

It's a good idea to think of the "stupidest possible" solution to a problem, before trying to get clever. Here's a fairly (but not completely) stupid algorithm.

RANDOM-LINEAR-CLASSIFIER($\mathcal{D}_n, k$)

1 **for** $j = 1$ **to** k
2 randomly sample $\left(\theta^{(j)}, \theta_0^{(j)}\right)$ from $(\mathbb{R}^d, \mathbb{R})$
3 $j^* = \arg\min_{j \in \{1,\ldots,k\}} \mathcal{E}_n\left(\theta^{(j)}, \theta_0^{(j)}\right)$
4 **return** $\left(\theta^{(j^*)}, \theta_0^{(j^*)}\right)$

A note about terminology and notation. The training data $\mathcal{D}_n$ is an input to the learning algorithm, and the output of this learning algorithm will be a hypothesis h, where h has parameters θ and θ_0. In contrast to θ and θ_0, the input k is a parameter of the learning algorithm itself; such parameters are often called *hyperparameters*.

The notation within the algorithm above might be new to you: $\arg\min_x f(x)$ means the value of x for which $f(x)$ is the smallest. Sometimes we write $\arg\min_{x \in \mathcal{X}} f(x)$ when we want to explicitly specify the set $\mathcal{X}$ of values of x over which we want to minimize.

Study Question: What do you think will be observed for $\mathcal{E}_n(h)$, where h is the hypothesis returned by RANDOM-LINEAR-CLASSIFIER, if this learning algorithm is run multiple times? And as k is increased?

Study Question: What properties of $\mathcal{D}_n$ do you think will have an effect on $\mathcal{E}_n(h)$?

5 Evaluating a learning algorithm

How should we evaluate the performance of a *classifier* h? The best method is to measure *test error* on data that was not used to train it.

How should we evaluate the performance of a *learning algorithm*? This is trickier. There are many potential sources of variability in the possible result of computing test error on a learned hypothesis h:

- Which particular *training examples* occurred in $\mathcal{D}_n$
- Which particular *testing examples* occurred in $\mathcal{D}_{n'}$
- Randomization inside the learning *algorithm* itself

Generally, we would like to execute the following process multiple times:

- Train on a new training set
- Evaluate resulting h on a testing set *that does not overlap the training set*

Doing this multiple times controls for possible poor choices of training set or unfortunate randomization inside the algorithm itself.

One concern is that we might need a lot of data to do this, and in many applications data is expensive or difficult to acquire. We can re-use data with *cross validation* (but it's harder to do theoretical analysis).

CROSS-VALIDATE($\mathcal{D}, k$)

1 divide $\mathcal{D}$ into k chunks $\mathcal{D}_1, \mathcal{D}_2, \ldots \mathcal{D}_k$ (of roughly equal size)
2 **for** $i = 1$ **to** k
3 train h_i on $\mathcal{D} \setminus \mathcal{D}_i$ (withholding chunk $\mathcal{D}_i$)
4 compute "test" error $\mathcal{E}_i(h_i)$ on withheld data $\mathcal{D}_i$
5 **return** $\frac{1}{k}\sum_{i=1}^{k} \mathcal{E}_i(h_i)$

It's very important to understand that cross-validation neither delivers nor evaluates a single particular hypothesis h. It evaluates the *algorithm* that produces hypotheses.

CHAPTER 3

The Perceptron

First of all, the coolest algorithm name! It is based on the 1943 model of neurons made by McCulloch and Pitts and by Hebb. It was developed by Rosenblatt in 1962. At the time, it was not interpreted as attempting to optimize any particular criteria; it was presented directly as an algorithm. There has, since, been a huge amount of study and analysis of its convergence properties and other aspects of its behavior.

Well, maybe "neocognitron," also the name of a real ML algorithm, is cooler.

1 Algorithm

Recall that we have a training dataset $\mathcal{D}_n$ with $x \in \mathbb{R}^d$, and $y \in \{-1, +1\}$. The Perceptron algorithm trains a binary classifier $h(x; \theta, \theta_0)$ using the following algorithm to find θ and θ_0 using (at most) τ iterative steps:

We use Greek letter τ here instead of T so we don't confuse it with transpose!

PERCEPTRON($\tau, \mathcal{D}_n$)

```
θ = [0  0  ···  0]^T
θ_0 = 0
for t = 1 to τ
    changed = False
    for i = 1 to n
        if y^(i) (θ^T x^(i) + θ_0) ⩽ 0
            θ = θ + y^(i) x^(i)
            θ_0 = θ_0 + y^(i)
            changed = True
    if NOT changed
        break
return θ, θ_0
```

Let's check dimensions. Remember that θ is $d \times 1$, $x^{(i)}$ is $d \times 1$, and $y^{(i)}$ is a scalar. Does everything match?

Intuitively, on each step, if the current hypothesis θ, θ_0 classifies example $x^{(i)}$ correctly, then no change is made. If it classifies $x^{(i)}$ incorrectly, then it moves θ, θ_0 so that it is "closer" to classifying $x^{(i)}, y^{(i)}$ correctly.

Note that if the algorithm ever steps once through every value of i without making an update, it will never make any further updates (this is true even if the "break" statement were removed; verify that you believe this!) and so it should just terminate at that point.

Study Question: *What is true about $\mathcal{E}_n$ if that happens?*

Example: Let h be the linear classifier defined by $\theta^{(0)} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \theta_0^{(0)} = 1$. The diagram below shows several points classified by h. However, in this case, h (represented by the bold line and normal vector $\theta^{(0)}$) misclassifies the point $x^{(1)} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$ which has label $y^{(1)} = 1$. Indeed,

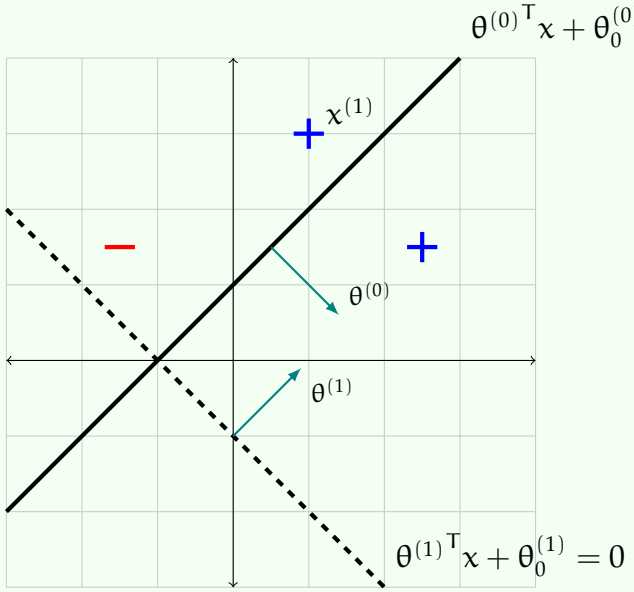
$$y^{(1)}\left(\theta^T x^{(1)} + \theta_0\right) = \begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 3 \end{bmatrix} + 1 = -1 < 0$$

By running an iteration of the Perceptron algorithm, we update

$$\theta^{(1)} = \theta^{(0)} + y^{(1)} x^{(1)} = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$$

$$\theta_0^{(1)} = \theta_0^{(0)} + y^{(1)} = 2$$

The new classifier (represented by the dashed line and normal vector $\theta^{(1)}$) now correctly classifies that point, but now makes a mistake on the negatively labeled point.



A really important fact about the perceptron algorithm is that, if there is a linear classifier with 0 training error, then for large enough τ this algorithm will (eventually) find it! We'll look at a proof of this in detail, next.

2 Offset

Sometimes, it can be easier to implement or analyze classifiers of the form

$$h(x; \theta) = \begin{cases} +1 & \text{if } \theta^T x > 0 \\ -1 & \text{otherwise.} \end{cases}$$

Without an explicit offset term (θ_0), this separator must pass through the origin, which may appear to be limiting. However, we can convert any problem involving a linear separator *with* offset into one with *no* offset (but of higher dimension)!

Consider the d-dimensional linear separator defined by $\theta = \begin{bmatrix}\theta_1 & \theta_2 & \cdots & \theta_d\end{bmatrix}$ and offset θ_0.

- for each data point $(x, y) \in \mathcal{D}_n$, append a coordinate with value +1 to x, yielding
$$x_{new} = \begin{bmatrix}x_1 & \cdots & x_d & +1\end{bmatrix}^T$$
- define
$$\theta_{new} = \begin{bmatrix}\theta_1 & \cdots & \theta_d & \theta_0\end{bmatrix}^T$$

Then,

$$\begin{aligned}\theta_{new}^T \cdot x_{new} &= \theta_1 x_1 + \cdots + \theta_d x_d + \theta_0 \cdot 1 \\ &= \theta^T x + \theta_0\end{aligned}$$

Thus, θ_{new} is an equivalent ($(d+1)$-dimensional) separator to our original, but with no offset.

Consider the data set:

$$\begin{aligned}X &= [[1], [2], [3], [4]] \\ Y &= [[+1], [+1], [-1], [-1]]\end{aligned}$$

It is linearly separable in $d = 1$ with $\theta = [-1]$ and $\theta_0 = 2.5$. But it is not linearly separable through the origin! Now, let

$$X_{new} = \left[\begin{bmatrix}1\\1\end{bmatrix}\begin{bmatrix}2\\1\end{bmatrix}\begin{bmatrix}3\\1\end{bmatrix}\begin{bmatrix}4\\1\end{bmatrix}\right]$$

This new dataset is separable through the origin, with $\theta_{new} = [-1, 2.5]^T$.

We can make a simplified version of the perceptron algorithm if we restrict ourselves to separators through the origin:

We list it here because this is the version of the algorithm we'll study in more detail.

PERCEPTRON-THROUGH-ORIGIN($\tau, \mathcal{D}_n$)

```
θ = [0 0 ··· 0]^T
for t = 1 to τ
    changed = False
    for i = 1 to n
        if y^(i) (θ^T x^(i)) ⩽ 0
            θ = θ + y^(i) x^(i)
            changed = True
    if NOT changed
        break
    return θ
```

3 Theory of the perceptron

Now, we'll say something formal about how well the perceptron algorithm really works. We start by characterizing the set of problems that can be solved perfectly by the perceptron algorithm, and then prove that, in fact, it can solve these problems. In addition, we provide a notion of what makes a problem difficult for perceptron and link that notion of difficulty to the number of updates the algorithm will make.

3.1 Linear separability

A training set $\mathcal{D}_n$ is *linearly separable* if there exist θ, θ_0 such that, for all $i = 1, 2, \ldots, n$:

$$y^{(i)} \left(\theta^T x^{(i)} + \theta_0 \right) > 0 \quad .$$

Another way to say that $\mathcal{D}_n$ is linearly separable is that there exists an h such that all predictions on the training set are correct,

$$h(x^{(i)}; \theta, \theta_0) = \left(\theta^T x^{(i)} + \theta_0 \right) = y^{(i)} \quad ,$$

in which case we call h a *linear separator*.

And, another way to say that $\mathcal{D}_n$ is linearly separable is that there exists an h of the form above such that the training error is zero,

$$\mathcal{E}_n(h) = 0 \quad .$$

3.2 Convergence theorem

The basic result about the perceptron is that, if the training data $\mathcal{D}_n$ is linearly separable, then the perceptron algorithm is guaranteed to find a linear separator, for large enough τ.

We will more specifically characterize the linear separability of the dataset by the *margin* of the separator. We'll start by defining the margin of a point with respect to a hyperplane.

First, recall that the signed distance from the hyperplane θ, θ_0 to a point x is

$$\frac{\theta^T x + \theta_0}{\|\theta\|} \quad .$$

Then, we'll define the *margin* of a *labeled point* (x, y) with respect to hyperplane θ, θ_0 to be

$$y \cdot \frac{\theta^T x + \theta_0}{\|\theta\|} \quad .$$

This quantity will be positive if and only if the point x is classified as y by the linear classifier represented by this hyperplane.

Study Question: What sign does the margin have if the point is incorrectly classified? Be sure you can explain why.

Now, the *margin* of a *dataset* $\mathcal{D}_n$ with respect to the hyperplane θ, θ_0 is the *minimum* margin of any point with respect to θ, θ_0:

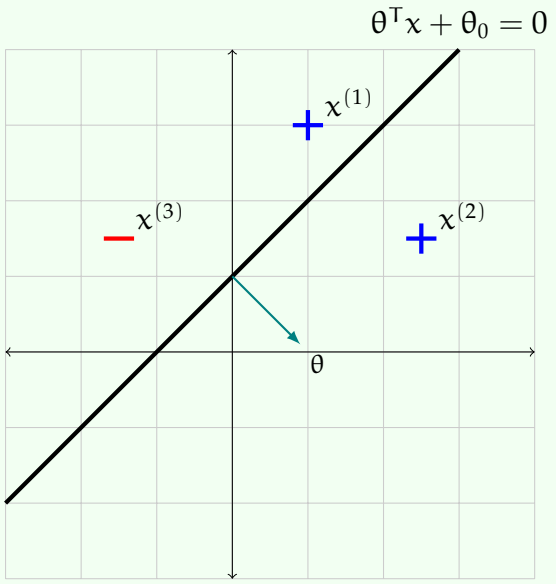
$$\min_i \left(y^{(i)} \cdot \frac{\theta^T x^{(i)} + \theta_0}{\|\theta\|} \right) \quad .$$

The margin is positive if and only if all of the points in the data-set are classified correctly. In that case (only!) it represents the distance from the hyperplane to the closest point.

If the training data is *not* linearly separable, the algorithm will not be able to tell you for sure, in finite time, that it is not linearly separable. There are other algorithms that can test for linear separability with run-times $O(n^{d/2})$ or $O(d^{2n})$ or $O(n^{d-1} \log n)$.

Example: Let h be the linear classifier defined by $\theta = \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \theta_0 = 1$.

The diagram below shows several points classified by h, one of which is misclassified. We compute the margin for each point:



$$y^{(1)} \cdot \frac{\theta^T x^{(1)} + \theta_0}{\|\theta\|} = 1 \cdot \frac{-2+1}{\sqrt{2}} = -\frac{\sqrt{2}}{2}$$

$$y^{(2)} \cdot \frac{\theta^T x^{(2)} + \theta_0}{\|\theta\|} = 1 \cdot \frac{1+1}{\sqrt{2}} = \sqrt{2}$$

$$y^{(3)} \cdot \frac{\theta^T x^{(3)} + \theta_0}{\|\theta\|} = -1 \cdot \frac{-3+1}{\sqrt{2}} = \sqrt{2}$$

Note that since point $x^{(1)}$ is misclassified, its margin is negative. Thus the margin for the whole data set is given by $-\frac{\sqrt{2}}{2}$.

Theorem 3.1 (Perceptron Convergence)**.** *For simplicity, we consider the case where the linear separator must pass through the origin, and τ is infinite. If the following conditions hold:*

(a) there exist θ^* and γ such that $\gamma > 0$, and $y^{(i)} \frac{\theta^{*T} x^{(i)}}{\|\theta^*\|} \geqslant \gamma$ for all $i = 1, \ldots, n$,

(b) all the examples have bounded magnitude: $\left\|x^{(i)}\right\| \leqslant R$ for all $i = 1, \ldots n$,

then the perceptron algorithm will make at most $\left(\frac{R}{\gamma}\right)^2$ updates to its starting hypothesis. At this point, its hypothesis will be a linear separator of the data.

Proof. We initialize $\theta^{(0)} = 0$, and let $\theta^{(k)}$ define our hyperplane after the perceptron algorithm has made k updates to its starting hypothesis. We are going to think about the angle between the hypothesis we have now, $\theta^{(k)}$ and the assumed good separator θ^*. Since they both go through the origin, if we can show that the angle between them is decreasing usefully across iterations, then we will get close to that separator.

So, let's think about the cos of the angle between them, and recall, by the definition of dot product:

$$\cos\left(\theta^{(k)}, \theta^*\right) = \frac{\theta^{(k)} \cdot \theta^*}{\|\theta^*\| \left\|\theta^{(k)}\right\|}$$

We'll divide this up into two factors,

$$\cos\left(\theta^{(k)}, \theta^*\right) = \left(\frac{\theta^{(k)} \cdot \theta^*}{\|\theta^*\|}\right) \cdot \left(\frac{1}{\left\|\theta^{(k)}\right\|}\right) \quad , \tag{3.1}$$

and start by focusing on the first factor.

Without loss of generality, assume that the k^{th} update occurs on the i^{th} example $\left(x^{(i)}, y^{(i)}\right)$.

$$\begin{aligned}
\frac{\theta^{(k)} \cdot \theta^*}{\|\theta^*\|} &= \frac{\left(\theta^{(k-1)} + y^{(i)} x^{(i)}\right) \cdot \theta^*}{\|\theta^*\|} \\
&= \frac{\theta^{(k-1)} \cdot \theta^*}{\|\theta^*\|} + \frac{y^{(i)} x^{(i)} \cdot \theta^*}{\|\theta^*\|} \\
&\geqslant \frac{\theta^{(k-1)} \cdot \theta^*}{\|\theta^*\|} + \gamma \\
&\geqslant k\gamma
\end{aligned}$$

where we have first applied the margin condition from (a) and then applied simple induction.

Now, we'll look at the second factor in equation 3.1. We note that since $\left(x^{(i)}, y^{(i)}\right)$ is classified incorrectly, $y^{(i)}\left(\theta^{(k-1)^T} x^{(i)}\right) \leqslant 0$. Thus,

$$\begin{aligned}
\left\|\theta^{(k)}\right\|^2 &= \left\|\theta^{(k-1)} + y^{(i)} x^{(i)}\right\|^2 \\
&= \left\|\theta^{(k-1)}\right\|^2 + 2y^{(i)} \theta^{(k-1)^T} x^{(i)} + \left\|x^{(i)}\right\|^2 \\
&\leqslant \left\|\theta^{(k-1)}\right\|^2 + R^2 \\
&\leqslant kR^2
\end{aligned}$$

where we have additionally applied the assumption from (b) and then again used simple induction.

Returning to the definition of the dot product, we have

$$\cos\left(\theta^{(k)}, \theta^*\right) = \frac{\theta^{(k)} \cdot \theta^*}{\left\|\theta^{(k)}\right\| \|\theta^*\|} = \left(\frac{\theta^{(k)} \cdot \theta^*}{\|\theta^*\|}\right) \frac{1}{\left\|\theta^{(k)}\right\|} \geqslant (k\gamma) \cdot \frac{1}{\sqrt{k}R} = \sqrt{k} \cdot \frac{\gamma}{R}$$

Since the value of the cosine is at most 1, we have

$$\begin{aligned}
1 &\geqslant \sqrt{k} \cdot \frac{\gamma}{R} \\
k &\leqslant \left(\frac{R}{\gamma}\right)^2 .
\end{aligned}$$

□

This result endows the margin γ of $\mathcal{D}_n$ with an operational meaning: when using the Perceptron algorithm for classification, at most $(R/\gamma)^2$ updates will be made, where R is an upper bound on the magnitude of the training vectors.

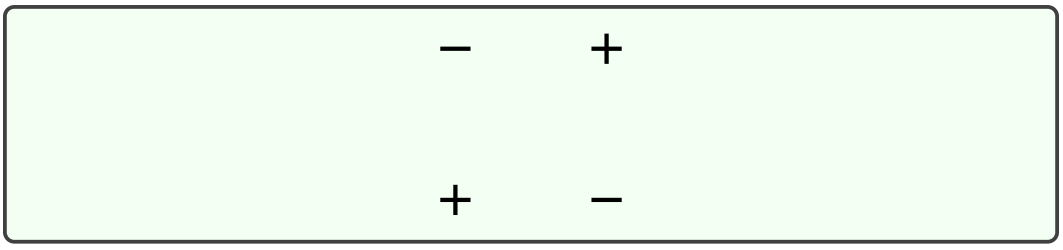
CHAPTER 4

Feature representation

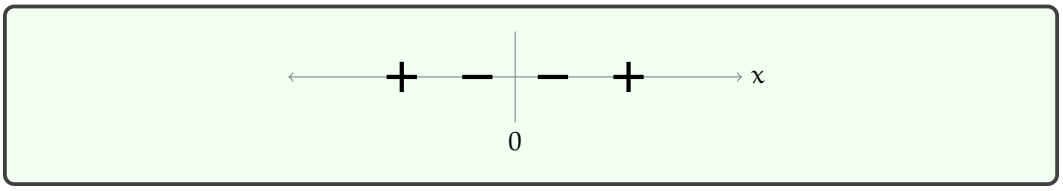
Linear classifiers are easy to work with and analyze, but they are a very restricted class of hypotheses. If we have to make a complex distinction in low dimensions, then they are unhelpful.

Our favorite illustrative example is the "exclusive or" (XOR) data set, the drosophila of machine-learning data sets:

D. Melanogaster is a species of fruit fly, used as a simple system in which to study genetics, since 1910.

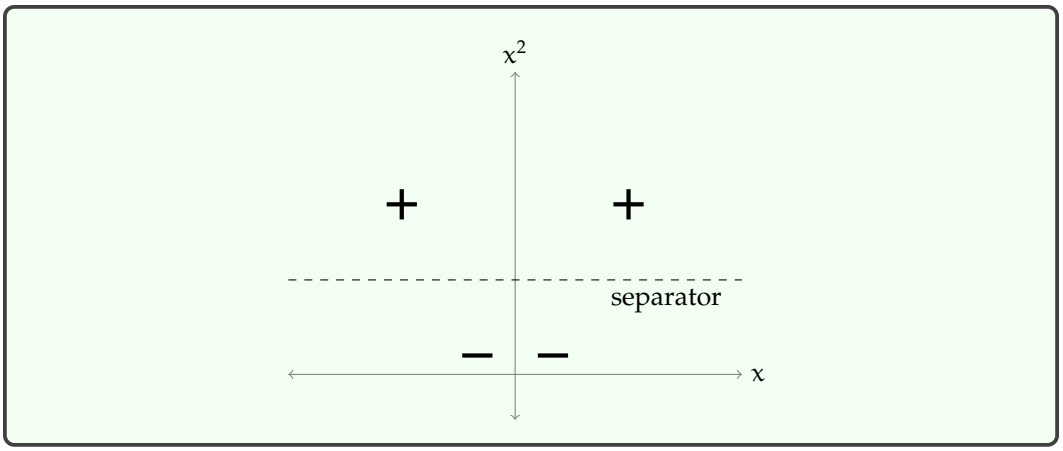


There is no linear separator for this two-dimensional dataset! But, we have a trick available: take a low-dimensional data set and move it, using a non-linear transformation into a higher-dimensional space, and look for a linear separator there. Let's look at an example data set that starts in 1-D:

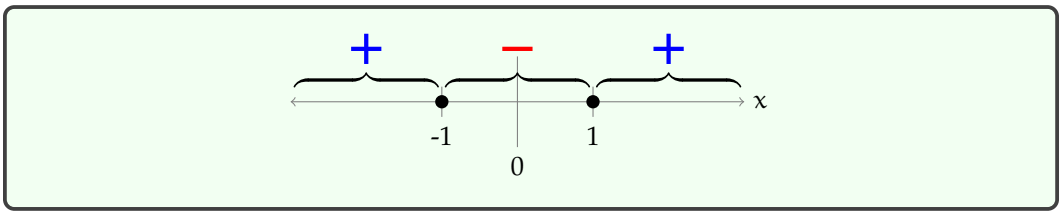


These points are not linearly separable, but consider the transformation $\phi(x) = [x, x^2]$. Putting the data in ϕ space, we see that it is now separable. There are lots of possible separators; we have just shown one of them here.

What's a linear separator for data in 1D? A point!



A linear separator in ϕ space is a nonlinear separator in the original space! Let's see how this plays out in our simple example. Consider the separator $x^2 - 1 = 0$, which labels the half-plane $x^2 - 1 > 0$ as positive. What separator does it correspond to in the original 1-D space? We have to ask the question: which x values have the property that $x^2 - 1 = 0$. The answer is $+1$ and -1, so those two points constitute our separator, back in the original space. And we can use the same reasoning to find the region of 1D space that is labeled positive by this separator.



This is a very general and widely useful strategy. It's the basis for *kernel methods*, a powerful technique that we unfortunately won't get to in this class, and can be seen as a motivation for multi-layer neural networks.

There are many different ways to construct ϕ. Some are relatively systematic and domain independent. We'll look at the *polynomial basis* in section 1 as an example of that. Others are directly related to the semantics (meaning) of the original features, and we construct them deliberately with our domain in mind. We'll explore that strategy in section 2.

1 Polynomial basis

If the features in your problem are already naturally numerical, one systematic strategy for constructing a new feature space is to use a *polynomial basis*. The idea is that, if you are using the kth-order basis (where k is a positive integer), you include a feature for every possible product of k different dimensions in your original input.

Here is a table illustrating the kth order polynomial basis for different values of k.

Order	$d = 1$	in general
0	$[1]$	$[1]$
1	$[1, x]$	$[1, x_1, \ldots, x_d]$
2	$[1, x, x^2]$	$[1, x_1, \ldots, x_d, x_1^2, x_1x_2, \ldots]$
3	$[1, x, x^2, x^3]$	$[1, x_1, \ldots, x_1^2, x_1x_2, \ldots, x_1x_2x_3, \ldots]$
$\vdots$	$\vdots$	$\vdots$

So, what if we try to solve the XOR problem using a polynomial basis as the feature transformation? We can just take our two-dimensional data and transform it into a higher-

dimensional data set, by applying ϕ. Now, we have a classification problem as usual, and we can use the perceptron algorithm to solve it.

Let's try it for $k = 2$ on our XOR problem. The feature transformation is

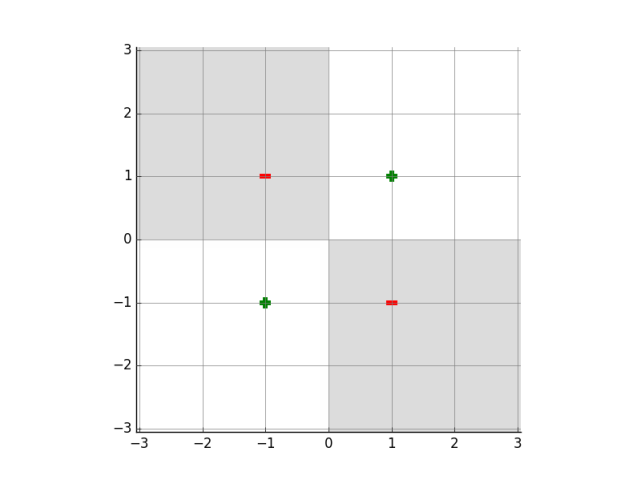
$$\phi((x_1, x_2)) = (1, x_1, x_2, x_1^2, x_1 x_2, x_2^2) \ .$$

Study Question: If we use perceptron to train a classifier after performing this feature transformation, would we lose any expressive power if we let $\theta_0 = 0$ (i.e. trained without offset instead of with offset)?

After 4 iterations, perceptron finds a separator with coefficients $\theta = (0, 0, 0, 0, 4, 0)$ and $\theta_0 = 0$. This corresponds to

$$0 + 0x_1 + 0x_2 + 0x_1^2 + 4x_1 x_2 + 0x_2^2 + 0 = 0$$

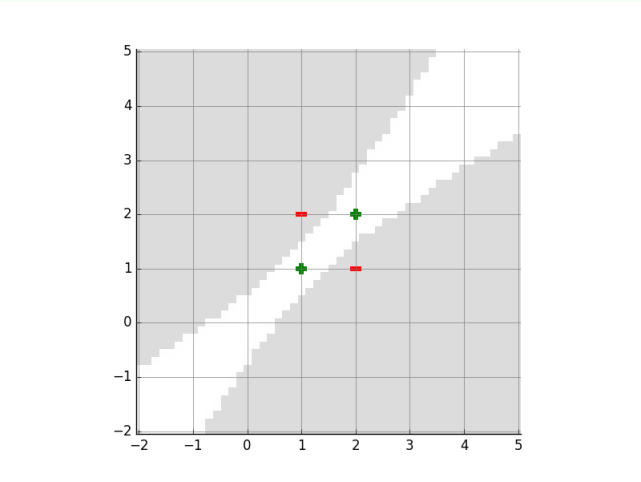
and is plotted below, with the gray shaded region classified as negative and the white region classified as positive:



Study Question: Be sure you understand why this high-dimensional hyperplane is a separator, and how it corresponds to the figure.

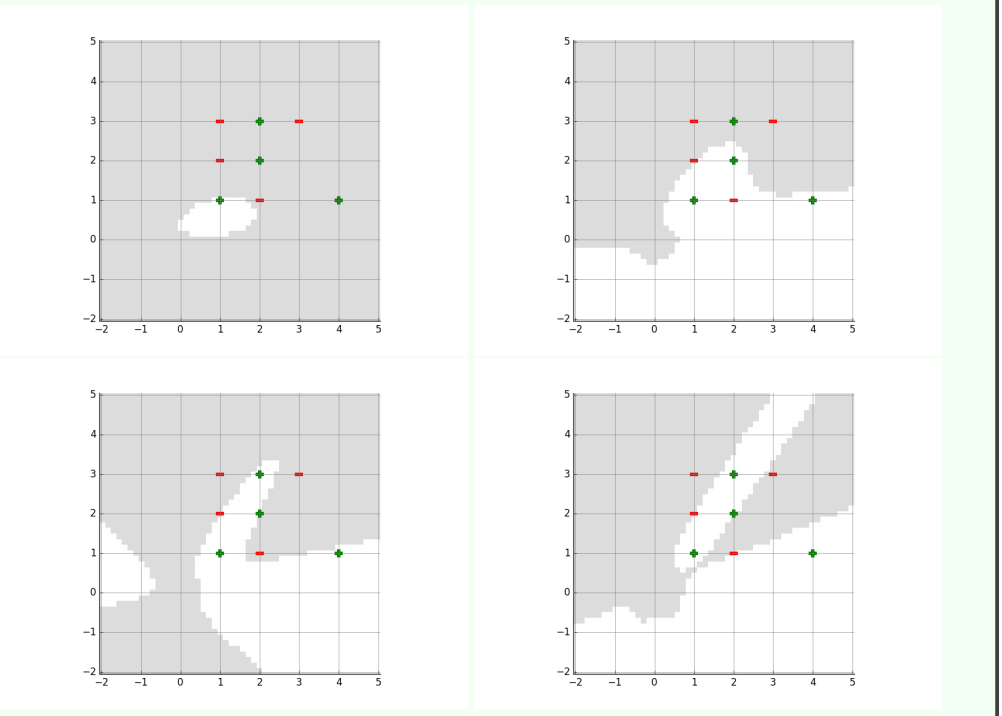
For fun, we show some more plots below. Here is the result of running perceptron on XOR, but where the data are put in a different place on the plane. After 65 mistakes (!) it arrives at these coefficients: $\theta = (1, -1, -1, -5, 11, -5)$, $\theta_0 = 1$, which generates this separator:

The jaggedness in the plotting of the separator is an artifact of a lazy lpk strategy for making these plots–the true curves are smooth.



Study Question: It takes many more iterations to solve this version. Apply knowledge of the convergence properties of the perceptron to understand why.

Here is a harder data set. After 200 iterations, we could not separate it with a second or third-order basis representation. Shown below are the results after 200 iterations for bases of order 2, 3, 4, and 5.



2 Hand-constructing features for real domains

In many machine-learning applications, we are given descriptions of the inputs with many different types of attributes, including numbers, words, and discrete features. An impor-

tant factor in the success of an ML application is the way that the features are chosen to be encoded by the human who is framing the learning problem.

2.1 Discrete features

Getting a good encoding of discrete features is particularly important. You want to create "opportunities" for the ML system to find the underlying regularities. Although there are machine-learning methods that have special mechanisms for handling discrete inputs, all the methods we consider in this class will assume the input vectors x are in $\mathbb{R}^d$. So, we have to figure out some reasonable strategies for turning discrete values into (vectors of) real numbers.

We'll start by listing some encoding strategies, and then work through some examples. Let's assume we have some feature in our raw data that can take on one of k discrete values.

- **Numeric** Assign each of these values a number, say $1.0/k, 2.0/k, \ldots, 1.0$. We might want to then do some further processing, as described in section 2.3. This is a sensible strategy *only* when the discrete values really do signify some sort of numeric quantity, so that these numerical values are meaningful.
- **Thermometer code** If your discrete values have a natural ordering, from $1, \ldots, k$, but not a natural mapping into real numbers, a good strategy is to use a vector of length k binary variables, where we convert discrete input value $0 < j \leqslant k$ into a vector in which the first j values are 1.0 and the rest are 0.0. This does not necessarily imply anything about the spacing or numerical quantities of the inputs, but does convey something about ordering.
- **Factored code** If your discrete values can sensibly be decomposed into two parts (say the "make" and "model" of a car), then it's best to treat those as two separate features, and choose an appropriate encoding of each one from this list.
- **One-hot code** If there is no obvious numeric, ordering, or factorial structure, then the best strategy is to use a vector of length k, where we convert discrete input value $0 < j \leqslant k$ into a vector in which all values are 0.0, except for the jth, which is 1.0.
- **Binary code** It might be tempting for the computer scientists among us to use some binary code, which would let us represent k values using a vector of length $\log k$. *This is a bad idea!* Decoding a binary code takes a lot of work, and by encoding your inputs this way, you'd be forcing your system to *learn* the decoding algorithm.

As an example, imagine that we want to encode blood types, which are drawn from the set $\{A+, A-, B+, B-, AB+, AB-, O+, O-\}$. There is no obvious linear numeric scaling or even ordering to this set. But there is a reasonable *factoring*, into two features: $\{A, B, AB, O\}$ and $\{+, -1\}$. And, in fact, we can reasonably factor the first group into $\{A, \text{not}A\}$, $\{B, \text{not}B\}$ So, here are two plausible encodings of the whole set:

It is sensible (according to Wikipedia!) to treat O as having neither feature A nor feature B.

- Use a 6-D vector, with two dimensions to encode each of the factors using a one-hot encoding.
- Use a 3-D vector, with one dimension for each factor, encoding its presence as 1.0 and absence as -1.0 (this is sometimes better than 0.0). In this case, $AB+$ would be $(1.0, 1.0, 1.0)$ and $O-$ would be $(-1.0, -1.0, -1.0)$.

Study Question: How would you encode $A+$ in both of these approaches?

2.2 Text

The problem of taking a text (such as a tweet or a product review, or even this document!) and encoding it as an input for a machine-learning algorithm is interesting and complicated. Much later in the class, we'll study sequential input models, where, rather than having to encode a text as a fixed-length feature vector, we feed it into a hypothesis word by word (or even character by character!).

There are some simpler encodings that work well for basic applications. One of them is the *bag of words* (BOW) model. The idea is to let d be the number of words in our vocabulary (either computed from the training set or some other body of text or dictionary). We will then make a binary vector (with values 1.0 and 0.0) of length d, where element j has value 1.0 if word j occurs in the document, and 0.0 otherwise.

2.3 Numeric values

If some feature is already encoded as a numeric value (heart rate, stock price, distance, etc.) then you should generally keep it as a numeric value. An exception might be a situation in which you know there are natural "breakpoints" in the semantics: for example, encoding someone's age in the US, you might make an explicit distinction between under and over 18 (or 21), depending on what kind of thing you are trying to predict. It might make sense to divide into discrete bins (possibly spacing them closer together for the very young) and to use a one-hot encoding for some sorts of medical situations in which we don't expect a linear (or even monotonic) relationship between age and some physiological features.

If you choose to leave a feature as numeric, it is typically useful to *scale* it, so that it tends to be in the range $[-1, +1]$. Without performing this transformation, if you have one feature with much larger values than another, it will take the learning algorithm a lot of work to find parameters that can put them on an equal basis. So, we might perform transformation $\phi(x) = \dfrac{x - \overline{x}}{\sigma}$, where $\overline{x}$ is the average of the $x^{(i)}$, and σ is the standard deviation of the $x^{(i)}$. The resulting feature values will have mean 0 and standard deviation 1. This transformation is sometimes called *standardizing* a variable .

Such standard variables are often known as "z-scores," for example, in the social sciences.

Then, of course, you might apply a higher-order polynomial-basis transformation to one or more groups of numeric features.

Study Question: Percy Eptron has a domain with 4 numeric input features, $(x_1, \ldots, x_4)$. He decides to use a representation of the form

$$\phi(x) = \text{PolyBasis}((x_1, x_2), 3) \frown \text{PolyBasis}((x_3, x_4), 3)$$

where $a \frown b$ means the vector a concatenated with the vector b. What is the dimension of Percy's representation? Under what assumptions about the original features is this a reasonable choice?

CHAPTER 5

Logistic regression

1 Machine learning as optimization

The perceptron algorithm was originally written down directly via cleverness and intuition, and later analyzed theoretically. Another approach to designing machine learning algorithms is to frame them as optimization problems, and then use standard optimization algorithms and implementations to actually find the hypothesis. Taking this approach will allow us to take advantage of a wealth of mathematical and algorithmic technique for understanding and solving optimization problems, which will allow us to move to hypothesis classes that are substantially more complex than linear separators.

We begin by writing down an *objective function* $J(\Theta)$, where Θ stands for *all* the parameters in our model. Note that we will sometimes write $J(\theta, \theta_0)$ because when studying linear classifiers, we have used these two names for parts of our whole collection of parameters, so $\Theta = (\theta, \theta_0)$. We also often write $J(\Theta; \mathcal{D})$ to make clear the dependence on the data $\mathcal{D}$. The objective function describes how we feel about possible hypotheses Θ: we will generally look for values for parameters Θ that minimize the objective function:

You can think about Θ^* here as "the theta that minimizes J".

$$\Theta^* = \arg\min_{\Theta} J(\Theta) \quad .$$

A very common form for an ML objective is

$$J(\Theta) = \left(\frac{1}{n} \sum_{i=1}^{n} \underbrace{\mathcal{L}(h(x^{(i)}; \Theta), y^{(i)})}_{\text{loss}} \right) + \underbrace{\lambda}_{\text{constant}} \underbrace{R(\Theta)}_{\text{regularizer}} \quad . \tag{5.1}$$

The *loss* tells us how unhappy we are about the prediction $h(x^{(i)}; \Theta)$ that Θ makes for $(x^{(i)}, y^{(i)})$. A common example is the 0-1 loss, introduced in chapter 1:

$$L_{01}(h(x; \Theta), y) = \begin{cases} 0 & \text{if } y = h(x; \Theta) \\ 1 & \text{otherwise} \end{cases} \quad ,$$

which gives a value of 0 for a correct prediction, and a 1 for an incorrect prediction. In the case of linear separators, this becomes:

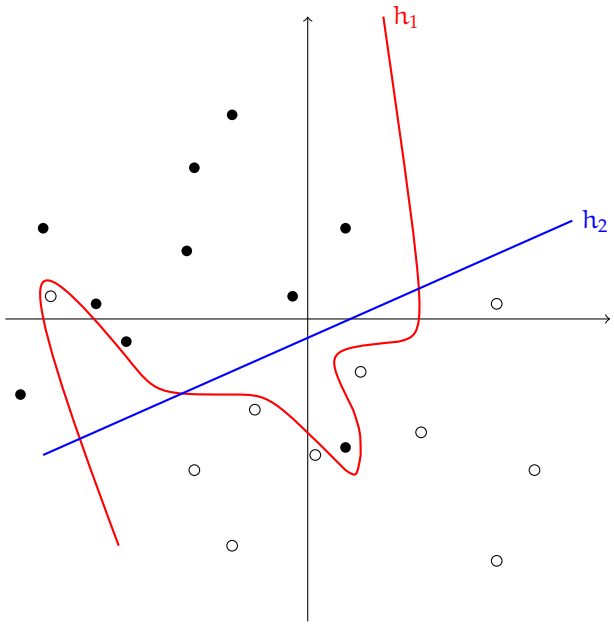
$$L_{01}(h(x; \theta, \theta_0), y) = \begin{cases} 0 & \text{if } y(\theta^T x + \theta_0) > 0 \\ 1 & \text{otherwise} \end{cases} \quad .$$

2 Regularization

If all we cared about was finding a hypothesis with small loss on the training data, we would have no need for regularization, and could simply omit the second term in the objective. But remember that our ultimate goal is to *perform well on input values that we haven't trained on!* It may seem that this is an impossible task, but humans and machine-learning methods do this successfully all the time. What allows *generalization* to new input values is a belief that there is an underlying regularity that governs both the training and testing data. We have already discussed one way to describe an assumption about such a regularity, which is by choosing a limited class of possible hypotheses. Another way to do this is to provide smoother guidance, saying that, within a hypothesis class, we prefer some hypotheses to others. The regularizer articulates this preference and the constant λ says how much we are willing to trade off loss on the training data versus preference over hypotheses.

This trade-off is illustrated in the figure below. Hypothesis h_1 has zero training loss, but is very complicated. Hypothesis h_2 mis-classifies two points, but is very simple. In absence of other beliefs about the solution, it is often better to prefer that the solution be "simpler," and so we might prefer h_2 over h_1, expecting it to perform better on future examples drawn from this same distribution. Another nice way of thinking about regularization is that we would like to prevent our hypothesis from being too dependent on the particular training data that we were given: we would like for it to be the case that if the training data were changed slightly, the hypothesis would not change by much.

To establish some vocabulary, we say that h_1 is *overfit* to the training data.



A common strategy for specifying a *regularizer* is to use the form

$$R(\Theta) = \left\|\Theta - \Theta_{prior}\right\|^2$$

when we have some idea in advance that θ ought to be near some value Θ_{prior}. In the absence of such knowledge a default is to *regularize toward zero*:

$$R(\Theta) = \|\Theta\|^2 \quad .$$

Learn about Bayesian methods in machine learning to see the theory behind this and cool results!

3 A new hypothesis class: linear logistic classifiers

For classification, it is natural to make predictions in $\{+1, -1\}$ and use the $0-1$ loss function. However, even for simple linear classifiers, it is very difficult to find values for θ, θ_0 that minimize simple training error

$$J(\theta, \theta_0) = \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}(\text{sign}(\theta^T x^{(i)} + \theta_0), y^{(i)}) \ .$$

This problem is NP-hard, which probably implies that solving the most difficult instances of this problem would require computation time *exponential* in the number of training examples, n.

The "probably" here is not because we're too lazy to look it up, but actually because of a fundamental unsolved problem in computer-science theory, known as "P vs NP."

What makes this a difficult optimization problem is its lack of "smoothness":

- There can be two hypotheses, (θ, θ_0) and (θ', θ_0'), where one is closer in parameter space to the optimal parameter values (θ^*, θ_0^*), but they make the same number of misclassifications so they have the same J value.
- All predictions are categorical: the classifier can't express a degree of certainty about whether a particular input x should have an associated value y.

For these reasons, if we are considering a hypothesis θ, θ_0 that makes five incorrect predictions, it is difficult to see how we might change θ, θ_0 so that it will perform better, which makes it difficult to design an algorithm that searches through the space of hypotheses for a good one.

For these reasons, we are going to investigate a new hypothesis class: *linear logistic classifiers*. These hypotheses are still parameterized by a d-dimensional vector θ and a scalar θ_0, but instead of making predictions in $\{+1, -1\}$, they generate real-valued outputs in the interval $(0, 1)$. A linear logistic classifier has the form

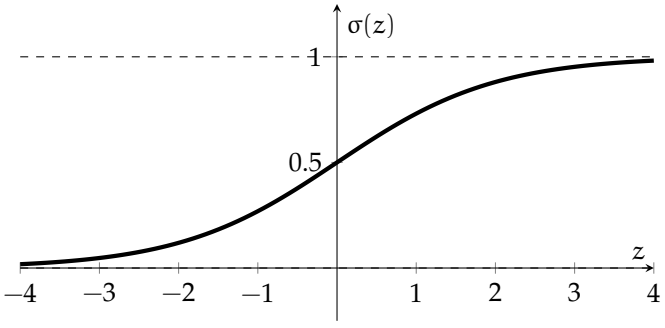
$$h(x; \theta, \theta_0) = \sigma(\theta^T x + \theta_0) \ .$$

This looks familiar! What's new?

The *logistic* function, also known as the *sigmoid* function, is defined as

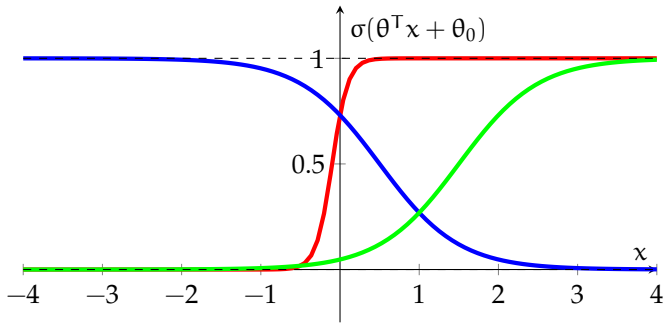
$$\sigma(z) = \frac{1}{1 + e^{-z}} \ ,$$

and plotted below, as a function of its input z. Its output can be interpreted as a probability, because for any value of z the output is in $(0, 1)$.



Study Question: Convince yourself the output of σ is always in the interval $(0, 1)$. Why can't it equal 0 or equal 1? For what value of z does $\sigma(z) = 0.5$?

What does a linear logistic classifier (LLC) look like? Let's consider the simple case where $d = 1$, so our input points simply lie along the x axis. The plot below shows LLCs for three different parameter settings: $\sigma(10x + 1)$, $\sigma(-2x + 1)$, and $\sigma(2x - 3)$.



Study Question: Which plot is which? What governs the steepness of the curve? What governs the x value where the output is equal to 0.5?

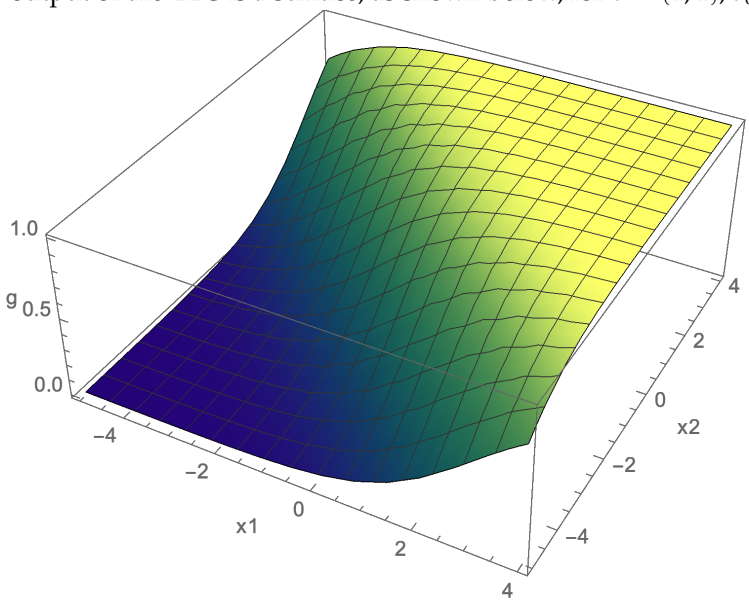
But wait! Remember that the definition of a classifier from chapter 2 is that it's a mapping from $\mathbb{R}^d \to \{-1, +1\}$ or to some other discrete set. So, then, it seems like an LLC is actually not a classifier!

Given an LLC, with an output value in $(0, 1)$, what should we do if we are forced to make a prediction in $\{+1, -1\}$? A default answer is to predict $+1$ if $\sigma(\theta^T x + \theta_0) > 0.5$ and -1 otherwise. The value 0.5 is sometimes called a *prediction threshold*.

In fact, for different problem settings, we might prefer to pick a different prediction threshold. The field of *decision theory* considers how to make this choice from the perspective of Bayesian reasoning. For example, if the consequences of predicting $+1$ when the answer should be -1 are much worse than the consequences of predicting -1 when the answer should be $+1$, then we might set the prediction threshold to be greater than 0.5.

Study Question: Using a prediction threshold of 0.5, for what values of x do each of the LLCs shown in the figure above predict $+1$?

When $d = 2$, then our inputs x lie in a two-dimensional space with axes x_1 and x_2, and the output of the LLC is a surface, as shown below, for $\theta = (1, 1), \theta_0 = 2$.



Study Question: Convince yourself that the set of points for which $\sigma(\theta^T x + \theta_0) = 0.5$, that is, the separator between positive and negative predictions with prediction threshold 0.5 is a line in (x_1, x_2) space. What particular line is it for the case in the figure above? How would the plot change for $\theta = (1, 1)$, but now with $\theta_0 = -2$? For $\theta = (-1, -1), \theta_0 = 2$?

4 Loss function for logistic classifiers

We have defined a class, LLC, of hypotheses whose outputs are in $(0, 1)$, but we have training data with y values in $\{+1, -1\}$. How can we define a loss function? Intuitively, we would like to have *low loss if we assign a low probability to the incorrect class.* We'll define a loss function, called *negative log-likelihood* (NLL), that does just this. In addition, it has the cool property that it extends nicely to the case where we would like to classify our inputs into more than two classes.

In order to simplify the description, we will assume that (or transform so that) the labels in the training data are $y \in \{0, 1\}$, enabling them to be interpreted as probabilities of being a member of the class of interest. We would like to pick the parameters of our classifier to maximize the probability assigned by the LCC to the correct y values, as specified in the training set. Letting guess $g^{(i)} = \sigma(\theta^T x^{(i)} + \theta_0)$, that probability is

Remember to be sure your y values have this form if you try to learn an LLC using NLL!!

$$\prod_{i=1}^{n} \begin{cases} g^{(i)} & \text{if } y^{(i)} = 1 \\ 1 - g^{(i)} & \text{otherwise} \end{cases} ,$$

under the assumption that our predictions are independent. This can be cleverly rewritten, when $y^{(i)} \in \{0, 1\}$, as

$$\prod_{i=1}^{n} {g^{(i)}}^{y^{(i)}} (1 - g^{(i)})^{1 - y^{(i)}} .$$

Study Question: Be sure you can see why these two expressions are the same.

Now, because products are kind of hard to deal with, and because the log function is monotonic, the θ, θ_0 that maximize the log of this quantity will be the same as the θ, θ_0 that maximize the original, so we can try to maximize

$$\sum_{i=1}^{n} \left(y^{(i)} \log g^{(i)} + (1 - y^{(i)}) \log(1 - g^{(i)}) \right) .$$

We can turn the maximization problem above into a minimization problem by taking the negative of the above expression, and write in terms of minimizing a loss

$$\sum_{i=1}^{n} \mathcal{L}_{\text{nll}}(g^{(i)}, y^{(i)})$$

where $\mathcal{L}_{\text{nll}}$ is the *negative log-likelihood* loss function:

$$\mathcal{L}_{\text{nll}}(\text{guess}, \text{actual}) = -\left(\text{actual} \cdot \log(\text{guess}) + (1 - \text{actual}) \cdot \log(1 - \text{guess})\right) .$$

This loss function is also sometimes referred to as the *log loss* or *cross entropy*.

You can use any base for the logarithm and it won't make any real difference. If we ask you for numbers, use log base e.

5 Logistic classification as optimization

We can finally put all these pieces together and develop an objective function for optimizing regularized negative log-likelihood for a linear logistic classifier. In fact, this process is usually called "logistic regression," so we'll call our objective J_{lr}, and define it as

That's a lot of fancy words!

$$J_{lr}(\theta, \theta_0; \mathcal{D}) = \left(\frac{1}{n} \sum_{i=1}^{n} \mathcal{L}_{nll}(\sigma(\theta^T x^{(i)} + \theta_0), y^{(i)}) \right) + \lambda \|\theta\|^2 \quad .$$

Study Question: Consider the case of linearly separable data. What will the θ values that optimize this objective be like if $\lambda = 0$? What will they be like if λ is very big? Try to work out an example in one dimension with two data points.

CHAPTER 6

Gradient Descent

In the previous chapter, we showed how to describe an interesting objective function for machine learning, but we need a way to find the optimal $\Theta^* = \arg\min_\Theta J(\Theta)$. There is an enormous, fascinating, literature on the mathematical and algorithmic foundations of optimization, but for this class, we will consider one of the simplest methods, called *gradient descent*.

Which you should consider studying some day!

Intuitively, in one or two dimensions, we can easily think of $J(\Theta)$ as defining a surface over Θ; that same idea extends to higher dimensions. Now, our objective is to find the Θ value at the lowest point on that surface. One way to think about gradient descent is that you start at some arbitrary point on the surface, look to see in which direction the "hill" goes down most steeply, take a small step in that direction, determine the direction of steepest descent from where you are, take another small step, etc.

Here's a very old-school humorous description of gradient descent and other optimization algorithms using analogies involving kangaroos: `ftp://ftp.sas.com/pub/neural/kangaroos.txt`

1 One dimension

We will start by considering gradient descent in one dimension. Assume $\Theta \in \mathbb{R}$, and that we know both $J(\Theta)$ and its first derivative with respect to Θ, $J'(\Theta)$. Here is pseudo-code for gradient descent on an arbitrary function f. Along with f and its gradient f', we have to specify the initial value for parameter Θ, a *step-size* parameter η, and an *accuracy* parameter ϵ:

1D-GRADIENT-DESCENT($\Theta_{init}, \eta, f, f', \epsilon$)
1 $\Theta^{(0)} = \Theta_{init}$
2 $t = 0$
3 **repeat**
4 $\quad t = t + 1$
5 $\quad \Theta^{(t)} = \Theta^{(t-1)} - \eta f'(\Theta^{(t-1)})$
6 **until** $|f(\Theta^{(t)}) - f(\Theta^{(t-1)})| < \epsilon$
7 **return** $\Theta^{(t)}$

Note that this algorithm terminates when the change in the function f is sufficiently small. There are many other reasonable ways to decide to terminate. These include the following.

- Stop after a fixed number of iterations T, i.e. when $t = T$.

- Stop when the change in the value of the parameter Θ is sufficiently small, i.e. when $\left|\Theta^{(t)} - \Theta^{(t-1)}\right| < \epsilon$.
- Stop when the derivative f' at the latest value of Θ is sufficiently small, i.e. when $\left|f'(\Theta^{(t)})\right| < \epsilon$.

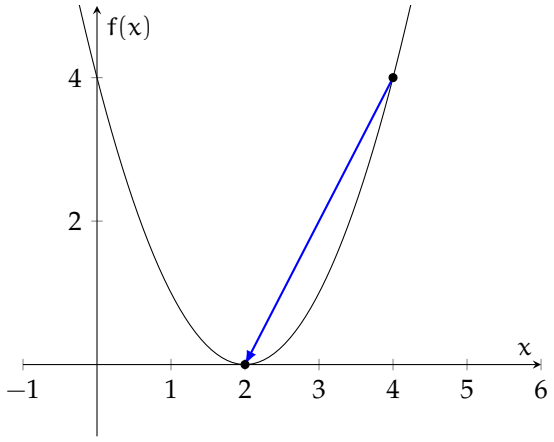
Study Question: In the list of possible stopping criteria for 1D-GRADIENT-DESCENT above, how do the final two potential criteria relate to each other?

Theorem 1.1. *Choose a small distance $\tilde{\epsilon} > 0$. If f is sufficiently "smooth" and convex, and if the step size η is sufficiently small, gradient descent will reach a point within $\tilde{\epsilon}$ of a global optimum Θ.*

A function is convex if the line segment between any two points on the graph of the function lies above or on the graph.

However, we must be careful when choosing the step size to prevent slow convergence, oscillation around the minimum, or divergence.

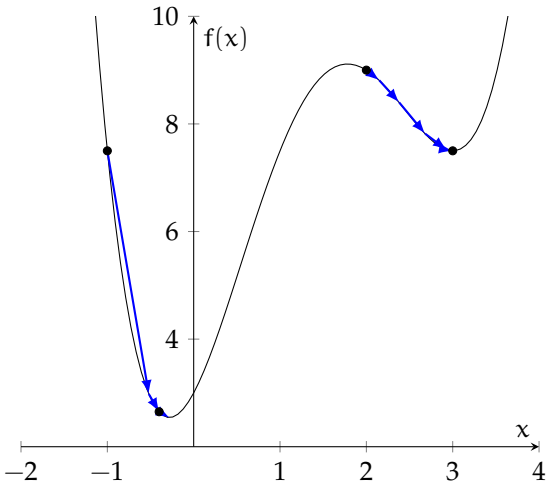
The following plot illustrates a convex function $f(x) = (x-2)^2$, starting gradient descent at $x_{\texttt{init}} = 4.0$ with a step-size of $1/2$. It is very well-behaved!



Study Question: What happens in this example with very small η? With very big η?

If f is non-convex, where gradient descent converges to depends on x_{init}. Given analytically defined derivatives for f, when gradient descent reaches a value of x where $f'(x) = 0$ and $f''(x) > 0$, this point is called a *local minimum* or *local optimum*. More generally, a local minimum is a point that is at least as low as all the points in some small area around it. A *global minimum* is a point that is at least as low as all the points in the function. A global minimum is also a local minimum, but a local minimum does not have to be a global minimum.

The plot below shows two different x_{init}, and two different resulting local optima.



2 Multiple dimensions

The extension to the case of multi-dimensional Θ is straightforward. Let's assume $\Theta \in \mathbb{R}^m$, so $f : \mathbb{R}^m \to \mathbb{R}$. The gradient of f with respect to Θ is

$$\nabla_\Theta f = \begin{bmatrix} \partial f/\partial \Theta_1 \\ \vdots \\ \partial f/\partial \Theta_m \end{bmatrix}$$

The algorithm remains the same, except that the update step in line 5 becomes

$$\Theta^{(t)} = \Theta^{(t-1)} - \eta \nabla_\Theta f(\Theta^{(t-1)})$$

and we have to change the termination criterion. The easiest thing is to keep the test in line 6 as $\left|f(\Theta^{(t)}) - f(\Theta^{(t-1)})\right| < \epsilon$, which is sensible no matter the dimensionality of Θ.

3 Application to logistic regression objective

We can now solve the optimization problem for our linear logistic classifier as formulated in chapter 5. We begin by stating the objective and the gradient necessary for doing gradient descent. In our problem where we are considering linear separators, the entire parameter vector is described by parameter vector θ and scalar θ_0 and so we will have to adjust them both and compute gradients of J with respect to each of them. The objective and gradient (note that we have replaced the constant λ with $\frac{\lambda}{2}$ for convenience), are, letting $g^{(i)} = \sigma(\theta^T x^{(i)} + \theta_0)$

The following step requires passing familiarity with matrix derivatives. A foolproof way of computing them is to compute partial derivative of J with respect to each component θ_i of θ.

$$J_{lr}(\theta, \theta_0) = \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}_{nll}(g^{(i)}, y^{(i)}) + \frac{\lambda}{2} \|\theta\|^2$$

$$\nabla_\theta J_{lr}(\theta, \theta_0) = \frac{1}{n} \sum_{i=1}^{n} \left(g^{(i)} - y^{(i)}\right) x^{(i)} + \lambda\theta$$

$$\frac{\partial J_{lr}(\theta, \theta_0)}{\partial \theta_0} = \frac{1}{n} \sum_{i=1}^{n} \left(g^{(i)} - y^{(i)}\right) \quad .$$

Note that $\nabla_\theta J_{lr}$ will be of shape $d \times 1$ and $\frac{\partial J_{lr}}{\partial \theta_0}$ will be a scalar since we have separated θ_0 from θ here.

Study Question: Convince yourself that the dimensions of all these quantities are correct, under the assumption that θ is $d \times 1$. How does d relate to m as discussed for Θ in the previous section?

Study Question: Compute $\nabla_\theta \|\theta\|^2$ by finding the vector of partial derivatives $(\partial \|\theta\|^2 / \partial\theta_1, \ldots, \partial \|\theta\|^2 / \partial\theta_d)$. What is the shape of $\nabla_\theta \|\theta\|^2$?

Study Question: Compute $\nabla_\theta \mathcal{L}_{nll}(\sigma(\theta^T x + \theta_0), y)$ by finding the vector of partial derivatives $(\partial \mathcal{L}_{nll}(\sigma(\theta^T x + \theta_0), y)/\partial\theta_1, \ldots, \partial \mathcal{L}_{nll}(\sigma(\theta^T x + \theta_0), y)/\partial\theta_d)$.

Study Question: Use these last two results to verify our derivation above.

Putting everything together, our gradient descent algorithm for logistic regression becomes

LR-GRADIENT-DESCENT($\theta_{init}, \theta_{0init}, \eta, \epsilon$)

1 $\theta^{(0)} = \theta_{init}$
2 $\theta_0^{(0)} = \theta_{0init}$
3 $t = 0$
4 **repeat**
5 $\quad t = t + 1$
6 $\quad \theta^{(t)} = \theta^{(t-1)} - \eta \left(\frac{1}{n} \sum_{i=1}^{n} \left(\sigma\left({\theta^{(t-1)}}^T x^{(i)} + \theta_0^{(t-1)} \right) - y^{(i)} \right) x^{(i)} + \lambda \theta^{(t-1)} \right)$
7 $\quad \theta_0^{(t)} = \theta_0^{(t-1)} - \eta \left(\frac{1}{n} \sum_{i=1}^{n} \left(\sigma\left({\theta^{(t-1)}}^T x^{(i)} + \theta_0^{(t-1)} \right) - y^{(i)} \right) \right)$
8 **until** $\left| J_{lr}(\theta^{(t)}, \theta_0^{(t)}) - J_{lr}(\theta^{(t-1)}, \theta_0^{(t-1)}) \right| < \epsilon$
9 **return** $\theta^{(t)}, \theta_0^{(t)}$

Study Question: Is it okay that λ doesn't appear in line 7?

4 Stochastic Gradient Descent

When the form of the gradient is a sum, rather than take one big(ish) step in the direction of the gradient, we can, instead, randomly select one term of the sum, and take a very small step in that direction. This seems sort of crazy, but remember that all the little steps would average out to the same direction as the big step if you were to stay in one place. Of course, you're not staying in that place, so you move, in expectation, in the direction of the gradient.

The word "stochastic" means probabilistic, or random; so does "aleatoric," which is a very cool word. Look up aleatoric music, sometime.

Most objective functions in machine learning can end up being written as a sum over data points, in which case, stochastic gradient descent (SGD) is implemented by picking a data point randomly out of the data set, computing the gradient as if there were only that one point in the data set, and taking a small step in the negative direction.

Let's assume our objective has the form

$$f(\Theta) = \sum_{i=1}^{n} f_i(\Theta) \quad .$$

Here is pseudocode for applying SGD to an objective f; it assumes we know the form of $\nabla_\Theta f_i$ for all i in $1 \ldots n$:

STOCHASTIC-GRADIENT-DESCENT($\Theta_{init}, \eta, f, \nabla_\Theta f_1, \ldots, \nabla_\Theta f_n, T$)

$\Theta^{(0)} = \Theta_{init}$
for $t = 1$ **to** T
    randomly select $i \in \{1, 2, \ldots, n\}$
    $\Theta^{(t)} = \Theta^{(t-1)} - \eta(t) \nabla_\Theta f_i(\Theta^{(t-1)})$
return $\Theta^{(t)}$

Note that now instead of a fixed value of η, η is indexed by the iteration of the algorithm, t. Choosing a good stopping criterion can be a little trickier for SGD than traditional gradient descent. Here we've just chosen to stop after a fixed number of iterations T.

For SGD to converge to a local optimum as t increases, the step size has to decrease as a function of time. The next result shows one step size sequence that works.

Theorem 4.1. *If f is convex, and $\eta(t)$ is a sequence satisfying*

$$\sum_{t=1}^{\infty} \eta(t) = \infty \quad \textit{and} \quad \sum_{t=1}^{\infty} \eta(t)^2 < \infty \ ,$$

then SGD converges with probability one *to the optimal Θ.*

We have left out some gnarly conditions in this theorem. Also, you can learn more about the subtle difference between "with probability one" and "always" by taking an advanced probability course.

One "legal" way of setting the step size is to make $\eta(t) = 1/t$ but people often use rules that decrease more slowly, and so don't strictly satisfy the criteria for convergence.

Study Question: If you start a long way from the optimum, would making $\eta(t)$ decrease more slowly tend to make you move more quickly or more slowly to the optimum?

There are multiple intuitions for why SGD might be a better choice algorithmically than regular GD (which is sometimes called *batch* GD (BGD)):

- If your f is actually non-convex, but has many shallow local optima that might trap BGD, then taking *samples* from the gradient at some point Θ might "bounce" you around the landscape and out of the local optima.
- Sometimes, optimizing f really well is not what we want to do, because it might overfit the training set; so, in fact, although SGD might not get lower training error than BGD, it might result in lower test error.
- BGD typically requires computing some quantity over every data point in a data set. SGD may perform well after visiting only some of the data. This behavior can be useful for very large data sets – in runtime and memory savings.

CHAPTER 7

Regression

Now we will turn to a slightly different form of machine-learning problem, called *regression*. It is still supervised learning, so our data will still have the form

"Regression," in common parlance, means moving backwards. But this is forward progress!

$$\mathcal{D}_n = \left\{ \left(x^{(1)}, y^{(1)} \right), \ldots, \left(x^{(n)}, y^{(n)} \right) \right\} \quad .$$

But now, instead of the y values being discrete, they will be real-valued, and so our hypotheses will have the form

$$h : \mathbb{R}^d \to \mathbb{R} \quad .$$

This is a good framework when we want to predict a numerical quantity, like height, stock value, etc., rather than to divide the inputs into categories.

The first step is to pick a loss function, to describe how to evaluate the quality of the predictions our hypothesis is making, when compared to the "target" y values in the data set. The choice of loss function is part of modeling your domain. In the absence of additional information about a regression problem, we typically use *squared error* (SE):

$$\text{Loss}(\text{guess}, \text{actual}) = (\text{guess} - \text{actual})^2 \quad .$$

It penalizes guesses that are too high the same amount as it penalizes guesses that are too low, and has a good mathematical justification in the case that your data are generated from an underlying linear hypothesis, but with Gaussian-distributed noise added to the y values.

We will consider the case of a linear hypothesis class,

$$h(x; \theta, \theta_0) = \theta^T x + \theta_0 \quad ,$$

remembering that we can get a rich class of hypotheses by performing a non-linear feature transformation before doing the regression. So, $\theta^T x + \theta_0$ is a linear function of x, but $\theta^T \phi(x) + \theta_0$ is a non-linear function of x if ϕ is a non-linear function of x.

We will treat regression as an optimization problem, in which, given a data set $\mathcal{D}$, we wish to find a linear hypothesis that minimizes *mean squared error*. Our objective is to find values for $\Theta = (\theta, \theta_0)$ that minimize

$$J(\theta, \theta_0) = \frac{1}{n} \sum_{i=1}^{n} \left(\theta^T x^{(i)} + \theta_0 - y^{(i)} \right)^2 \quad ,$$

resulting in the solution:

$$\theta^*, \theta_0^* = \arg\min_{\theta,\theta_0} J(\theta, \theta_0) \quad . \tag{7.1}$$

1 Analytical solution: ordinary least squares

One very interesting aspect of the problem of finding a linear hypothesis that minimizes mean squared error (this general problem is often called *ordinary least squares* (OLS)) is that we can find a closed-form formula for the answer!

What does "closed form" mean? Generally, that it involves direct evaluation of a mathematical expression using a fixed number of "typical" operations (like arithmetic operations, trig functions, powers, etc.). So equation 7.1 is not in closed form, because it's not at all clear what operations one needs to perform to find the solution.

Everything is easier to deal with if we assume that the $x^{(i)}$ have been augmented with an extra input dimension (feature) that always has value 1, so we may ignore θ_0. (See chapter 3, section 2 for a reminder about this strategy). This is what we will assume in this section. In this case, the objective becomes

$$J(\theta) = \frac{1}{n} \sum_{i=1}^{n} \left(\theta^T x^{(i)} - y^{(i)} \right)^2 \quad .$$

We will approach this just like a minimization problem from calculus homework: take the derivative of J with respect to θ, set it to zero, and solve for θ. There is an additional step required, to check that the resulting θ is a minimum (rather than a maximum or an inflection point) but we won't work through that here. It is possible to approach this problem by:

- Finding $\partial J / \partial \theta_k$ for k in $1, \ldots, d$,
- Constructing a set of k equations of the form $\partial J / \partial \theta_k = 0$, and
- Solving the system for values of θ_k.

We will use d here for the total number of features in each $x^{(i)}$, including the added 1.

That works just fine. To get practice for applying techniques like this to more complex problems, we will work through a more compact (and cool!) matrix view.

Study Question: Work through this and check your answer against ours below.

We can think of our training data in terms of matrices X and Y, where each column of X is an example, and each "column" of Y is the corresponding target output value:

$$X = \begin{bmatrix} x_1^{(1)} & \ldots & x_1^{(n)} \\ \vdots & \ddots & \vdots \\ x_d^{(1)} & \ldots & x_d^{(n)} \end{bmatrix} \quad Y = \begin{bmatrix} y^{(1)} & \ldots & y^{(n)} \end{bmatrix} \quad .$$

Study Question: What are the dimensions of X and Y?

In most textbooks, they think of an individual example $x^{(i)}$ as a row, rather than a column. So that we get an answer that will be recognizable to you, we are going to define a new matrix and vector, $\tilde{X}$ and $\tilde{Y}$, which are just transposes of our X and Y, and then work with them:

$$\tilde{X} = X^T = \begin{bmatrix} x_1^{(1)} & \ldots & x_d^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(n)} & \ldots & x_d^{(n)} \end{bmatrix} \quad \tilde{Y} = Y^T = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(n)} \end{bmatrix} \quad .$$

Study Question: What are the dimensions of $\tilde{X}$ and $\tilde{Y}$?

Now we can write

$$J(\theta) = \frac{1}{n} \underbrace{(\tilde{X}\theta - \tilde{Y})^T}_{1\times n} \underbrace{(\tilde{X}\theta - \tilde{Y})}_{n\times 1} = \frac{1}{n} \sum_{i=1}^{n} \left(\left(\sum_{j=1}^{d} \tilde{X}_{ij}\theta_j \right) - \tilde{Y}_i \right)^2$$

and using facts about matrix/vector calculus, we get

$$\nabla_\theta J = \frac{2}{n} \underbrace{\tilde{X}^T}_{d\times n} \underbrace{(\tilde{X}\theta - \tilde{Y})}_{n\times 1} \ .$$

Setting to 0 and solving, we get:

$$\begin{aligned} \frac{2}{n}\tilde{X}^T(\tilde{X}\theta - \tilde{Y}) &= 0 \\ \tilde{X}^T\tilde{X}\theta - \tilde{X}^T\tilde{Y} &= 0 \\ \tilde{X}^T\tilde{X}\theta &= \tilde{X}^T\tilde{Y} \\ \theta &= (\tilde{X}^T\tilde{X})^{-1}\tilde{X}^T\tilde{Y} \end{aligned}$$

And the dimensions work out!

$$\theta = \underbrace{\left(\tilde{X}^T\tilde{X}\right)^{-1}}_{d\times d} \underbrace{\tilde{X}^T}_{d\times n} \underbrace{\tilde{Y}}_{n\times 1}$$

So, given our data, we can directly compute the linear regression that minimizes mean squared error. That's pretty awesome!

2 Regularizing linear regression

Well, actually, there are some kinds of trouble we can get into. What if $(\tilde{X}^T\tilde{X})$ is not invertible?

Study Question: Consider, for example, a situation where the data-set is just the same point repeated twice: $x^{(1)} = x^{(2)} = (1, 2)^T$. What is $\tilde{X}$ in this case? What is $\tilde{X}^T\tilde{X}$? What is $(\tilde{X}^T\tilde{X})^{-1}$?

Another kind of problem is *overfitting*: we have formulated an objective that is just about fitting the data as well as possible, but as we discussed in the context of logistic regression, we might also want to *regularize* to keep the hypothesis from getting *too* attached to the data.

We address both the problem of not being able to invert $(\tilde{X}^T\tilde{X})^{-1}$ and the problem of overfitting using a mechanism called *ridge regression*. We add a regularization term $\|\theta\|^2$ to the OLS objective, with trade-off parameter λ.

Study Question: When we add a regularizer of the form $\|\theta\|^2$, what is our most "preferred" value of θ, in the absence of any data?

Here is the ridge regression objective function:

$$J_{\text{ridge}}(\theta, \theta_0) = \frac{1}{n} \sum_{i=1}^{n} \left(\theta^T x^{(i)} + \theta_0 - y^{(i)} \right)^2 + \lambda\|\theta\|^2$$

Larger λ values pressure θ values to be near zero. Note that we don't penalize θ_0; intuitively, θ_0 is what "floats" the regression surface to the right level for the data you have,

and so you shouldn't make it harder to fit a data set where the y values tend to be around one million than one where they tend to be around one. The other parameters control the orientation of the regression surface, and we prefer it to have a not-too-crazy orientation.

There is an analytical expression for the θ, θ_0 values that minimize J_{ridge}, but it's a little bit more complicated to derive than the solution for OLS because θ_0 needs special treatment. If we decide not to treat θ_0 specially (so we add a 1 feature to our input vectors), then we get:

$$\nabla_\theta J_{\text{ridge}} = \frac{2}{n}\tilde{X}^T(\tilde{X}\theta - \tilde{Y}) + 2\lambda\theta \quad .$$

Setting to 0 and solving, we get:

$$\begin{aligned}
\frac{2}{n}\tilde{X}^T(\tilde{X}\theta - \tilde{Y}) + 2\lambda\theta &= 0 \\
\frac{1}{n}\tilde{X}^T\tilde{X}\theta - \frac{1}{n}\tilde{X}^T\tilde{Y} + \lambda\theta &= 0 \\
\frac{1}{n}\tilde{X}^T\tilde{X}\theta + \lambda\theta &= \frac{1}{n}\tilde{X}^T\tilde{Y} \\
\tilde{X}^T\tilde{X}\theta + n\lambda\theta &= \tilde{X}^T\tilde{Y} \\
(\tilde{X}^T\tilde{X} + n\lambda I)\theta &= \tilde{X}^T\tilde{Y} \\
\theta &= (\tilde{X}^T\tilde{X} + n\lambda I)^{-1}\tilde{X}^T\tilde{Y}
\end{aligned}$$

Whew! So,

$$\theta_{\text{ridge}} = \left(\tilde{X}^T\tilde{X} + n\lambda I\right)^{-1}\tilde{X}^T\tilde{Y}$$

which becomes invertible when $\lambda > 0$.

This is called "ridge" regression because we are adding a "ridge" of $n\lambda$ values along the diagonal of the matrix before inverting it.

Study Question: Derive this version of the ridge regression solution.

Talking about regularization In machine learning in general, not just regression, it is useful to distinguish two ways in which a hypothesis $h \in \mathcal{H}$ might contribute to errors on test data. We have

Structural error: This is error that arises because there is no hypothesis $h \in \mathcal{H}$ that will perform well on the data, for example because the data was really generated by a sin wave but we are trying to fit it with a line.

Estimation error: This is error that arises because we do not have enough data (or the data are in some way unhelpful) to allow us to choose a good $h \in \mathcal{H}$.

When we increase λ, we tend to increase structural error but decrease estimation error, and vice versa.

There are technical definitions of these concepts that are studied in more advanced treatments of machine learning. Structural error is referred to as *bias* and estimation error is referred to as *variance*.

Study Question: Consider using a polynomial basis of order k as a feature transformation ϕ on your data. Would increasing k tend to increase or decrease structural error? What about estimation error?

3 Optimization via gradient descent

Inverting the $d \times d$ matrix $\left(\tilde{X}^T\tilde{X}\right)$ takes $O(d^3)$ time, which makes the analytic solution impractical for large d. If we have high-dimensional data, we can fall back on gradient descent.

Well, actually, Gauss-Jordan elimination, a popular algorithm, takes $O(d^3)$ arithmetic operations, but the bit complexity of the intermediate results can grow exponentially! There are other algorithms with polynomial bit complexity. (If this just made no sense to you, don't worry.)

Study Question: Why is having large n not as much of a computational problem as having large d?

Recall the ridge objective

$$J_{\text{ridge}}(\theta, \theta_0) = \frac{1}{n} \sum_{i=1}^{n} \left(\theta^T x^{(i)} + \theta_0 - y^{(i)} \right)^2 + \lambda \|\theta\|^2$$

and its gradient with respect to θ

$$\nabla_\theta J = \frac{2}{n} \sum_{i=1}^{n} \left(\theta^T x^{(i)} + \theta_0 - y^{(i)} \right) x^{(i)} + 2\lambda\theta$$

and partial derivative with respect to θ_0

$$\frac{\partial J}{\partial \theta_0} = \frac{2}{n} \sum_{i=1}^{n} \left(\theta^T x^{(i)} + \theta_0 - y^{(i)} \right) \quad .$$

Armed with these derivatives, we can do gradient descent, using the regular or stochastic gradient methods from chapter 6.

Even better, the objective functions for OLS and ridge regression are *convex*, which means they have only one minimum, which means, with a small enough step size, gradient descent is *guaranteed* to find the optimum.

CHAPTER 8

Neural Networks

Unless you live under a rock with no internet access, you've been hearing a lot about "neural networks." Now that we have several useful machine-learning concepts (hypothesis classes, classification, regression, gradient descent, regularization, etc.) we are completely well equipped to understand neural networks in detail.

This is, in some sense, the "third wave" of neural nets. The basic idea is founded on the 1943 model of neurons of McCulloch and Pitts and learning ideas of Hebb. There was a great deal of excitement, but not a lot of practical success: there were good training methods (e.g., perceptron) for linear functions, and interesting examples of non-linear functions, but no good way to train non-linear functions from data. Interest died out for a while, but was re-kindled in the 1980s when several people came up with a way to train neural networks with "back-propagation," which is a particular style of implementing gradient descent, which we will study here. By the mid-90s, the enthusiasm waned again, because although we could train non-linear networks, the training tended to be slow and was plagued by a problem of getting stuck in local optima. Support vector machines (SVMs) (regularization of high-dimensional hypotheses by seeking to maximize the margin) and kernel methods (an efficient and beautiful way of using feature transformations to non-linearly transform data into a higher-dimensional space) provided reliable learning methods with guaranteed convergence and no local optima.

As with many good ideas in science, the basic idea for how to train non-linear neural networks with gradient descent, was independently developed by more than one researcher.

However, during the SVM enthusiasm, several groups kept working on neural networks, and their work, in combination with an increase in available data and computation, has made them rise again. They have become much more reliable and capable, and are now the method of choice in many applications. There are many, many variations of neural networks, which we can't even begin to survey. We will study the core "feed-forward" networks with "back-propagation" training, and then, in later chapters, address some of the major advances beyond this core.

The number increases daily, as may be seen on `arxiv.org`.

We can view neural networks from several different perspectives:

View 1: An application of stochastic gradient descent for classification and regression with a potentially very rich hypothesis class.

View 2: A brain-inspired network of neuron-like computing elements that learn distributed representations.

View 3: A method for building applications that make predictions based on huge amounts

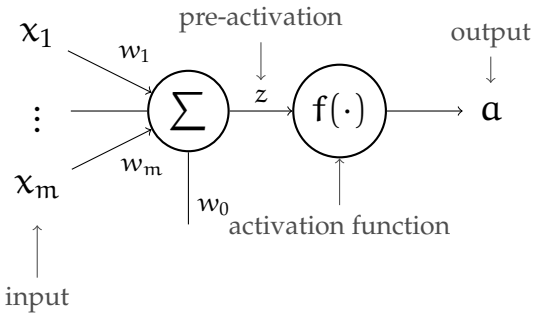
of data in very complex domains.

We will mostly take view 1, with the understanding that the techniques we develop will enable the applications in view 3. View 2 was a major motivation for the early development of neural networks, but the techniques we will study do not seem to actually account for the biological learning processes in brains.

Some prominent researchers are, in fact, working hard to find analogues of these methods in the brain

1 Basic element

The basic element of a neural network is a "neuron," pictured schematically below. We will also sometimes refer to a neuron as a "unit" or "node."



It is a non-linear function of an input vector $x \in \mathbb{R}^m$ to a single output value $a \in \mathbb{R}$. It is parameterized by a vector of *weights* $(w_1, \ldots, w_m) \in \mathbb{R}^m$ and an *offset* or *threshold* $w_0 \in \mathbb{R}$. In order for the neuron to be non-linear, we also specify an *activation function* $f : \mathbb{R} \to \mathbb{R}$, which can be the identity ($f(x) = x$, in that case the neuron is a linear function of x), but can also be any other function, though we will only be able to work with it if it is differentiable.

Sorry for changing our notation here. We were using d as the dimension of the input, but we are trying to be consistent here with many other accounts of neural networks. It is impossible to be consistent with all of them though—there are many different ways of telling this story.

The function represented by the neuron is expressed as:

$$a = f(z) = f\left(\left(\sum_{j=1}^{m} x_j w_j\right) + w_0\right) = f(w^T x + w_0) \quad .$$

Before thinking about a whole network, we can consider how to train a single unit. Given a loss function $L(\text{guess}, \text{actual})$ and a dataset $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$, we can do (stochastic) gradient descent, adjusting the weights w, w_0 to minimize

This should remind you of our θ and θ_0 for linear models.

$$J(w, w_0) = \sum_i L\left(NN(x^{(i)}; w, w_0), y^{(i)}\right) \quad .$$

where NN is the output of our neural net for a given input.

We have already studied two special cases of the neuron: linear logistic classifiers (LLC) with NLL loss and regressors with quadratic loss! The activation function for the LLC is $f(x) = \sigma(x)$ and for linear regression it is simply $f(x) = x$.

Study Question: Just for a single neuron, imagine for some reason, that we decide to use activation function $f(z) = e^z$ and loss function $L(\text{guess}, \text{actual}) = (\text{guess} - \text{actual})^2$. Derive a gradient descent update for w and w_0.

2 Networks

Now, we'll put multiple neurons together into a *network*. A neural network in general takes in an input $x \in \mathbb{R}^m$ and generates an output $a \in \mathbb{R}^n$. It is constructed out of multiple

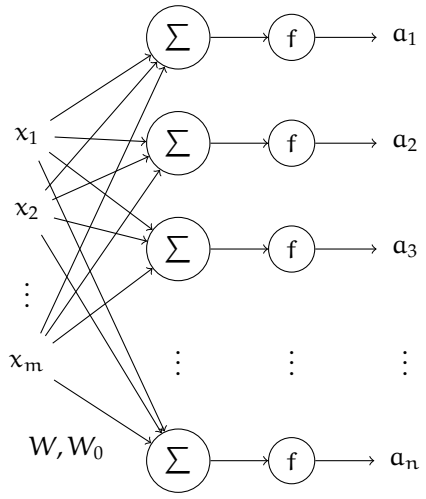
neurons; the inputs of each neuron might be elements of x and/or outputs of other neurons. The outputs are generated by n *output units*.

In this chapter, we will only consider *feed-forward* networks. In a feed-forward network, you can think of the network as defining a function-call graph that is *acyclic*: that is, the input to a neuron can never depend on that neuron's output. Data flows, one way, from the inputs to the outputs, and the function computed by the network is just a composition of the functions computed by the individual neurons.

Although the graph structure of a neural network can really be anything (as long as it satisfies the feed-forward constraint), for simplicity in software and analysis, we usually organize them into *layers*. A layer is a group of neurons that are essentially "in parallel": their inputs are outputs of neurons in the previous layer, and their outputs are the input to the neurons in the next layer. We'll start by describing a single layer, and then go on to the case of multiple layers.

2.1 Single layer

A *layer* is a set of units that, as we have just described, are not connected to each other. The layer is called *fully connected* if, as in the diagram below, the inputs to each unit in the layer are the same (i.e. $x_1, x_2, \ldots x_m$ in this case). A layer has input $x \in \mathbb{R}^m$ and output (also known as *activation*) $a \in \mathbb{R}^n$.



Since each unit has a vector of weights and a single offset, we can think of the weights of the whole layer as a matrix, W, and the collection of all the offsets as a vector W_0. If we have m inputs, n units, and n outputs, then

- W is an $m \times n$ matrix,
- W_0 is an $n \times 1$ column vector,
- X, the input, is an $m \times 1$ column vector,
- $Z = W^T X + W_0$, the *pre-activation*, is an $n \times 1$ column vector,
- A, the *activation*, is an $n \times 1$ column vector,

and the output vector is

$$A = f(Z) = f(W^T X + W_0) \quad .$$

The activation function f is applied element-wise to the pre-activation values Z.

What can we do with a single layer? We have already seen single-layer networks, in the form of linear separators and linear regressors. All we can do with a single layer is make a linear hypothesis. The whole reason for moving to neural networks is to move in the direction of *non-linear* hypotheses. To do this, we will have to consider multiple layers, where we can view the last layer as still being a linear classifier or regressor, but where we interpret the previous layers as learning a non-linear feature transformation $\phi(x)$, rather than having us hand-specify it.

We have used a step or sigmoid function to transform the linear output value for classification, but it's important to be clear that the resulting *separator* is still linear.

2.2 Many layers

A single neural network generally combines multiple layers, most typically by feeding the outputs of one layer into the inputs of another layer.

We have to start by establishing some nomenclature. We will use l to name a layer, and let m^l be the number of inputs to the layer and n^l be the number of outputs from the layer. Then, W^l and W_0^l are of shape $m^l \times n^l$ and $n^l \times 1$, respectively. Note that the input to layer l is the output from layer $l-1$, so we have $m^l = n^{l-1}$, and as a result A^{l-1} is of shape $m^l \times 1$, or equivalently $n^{l-1} \times 1$. Let f^l be the activation function of layer l. Then, the pre-activation outputs are the $n^l \times 1$ vector

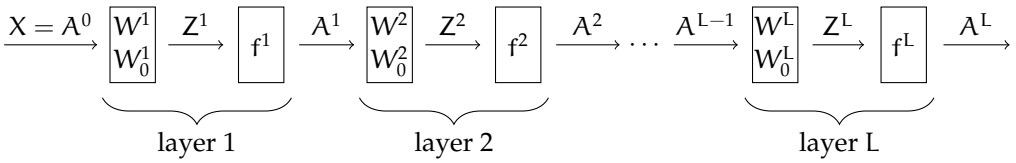
$$Z^l = {W^l}^T A^{l-1} + W_0^l$$

and the activation outputs are simply the $n^l \times 1$ vector

$$A^l = f^l(Z^l) \ .$$

It is technically possible to have different activation functions within the same layer, but, again, for convenience in specification and implementation, we generally have the same activation function within a layer.

Here's a diagram of a many-layered network, with two blocks for each layer, one representing the linear part of the operation and one representing the non-linear activation function. We will use this structural decomposition to organize our algorithmic thinking and implementation.



3 Choices of activation function

There are many possible choices for the activation function. We will start by thinking about whether it's really necessary to have an f at all.

What happens if we let f be the identity? Then, in a network with L layers (we'll leave out W_0 for simplicity, but keeping it wouldn't change the form of this argument),

$$A^L = {W^L}^T A^{L-1} = {W^L}^T {W^{L-1}}^T \cdots {W^1}^T X \ .$$

So, multiplying out the weight matrices, we find that

$$A^L = W^{\text{total}} X \ ,$$

which is a *linear* function of X! Having all those layers did not change the representational capacity of the network: the non-linearity of the activation function is crucial.

Study Question: Convince yourself that any function representable by any number of linear layers (where f is the identity function) can be represented by a single layer.

Now that we are convinced we need a non-linear activation, let's examine a few common choices.

Step function:

$$\text{step}(z) = \begin{cases} 0 & \text{if } z < 0 \\ 1 & \text{otherwise} \end{cases}$$

Rectified linear unit (ReLU):

$$\text{ReLU}(z) = \begin{cases} 0 & \text{if } z < 0 \\ z & \text{otherwise} \end{cases} = \max(0, z)$$

Sigmoid function: Also known as a *logistic* function, can be interpreted as probability, because for any value of z the output is in $(0, 1)$

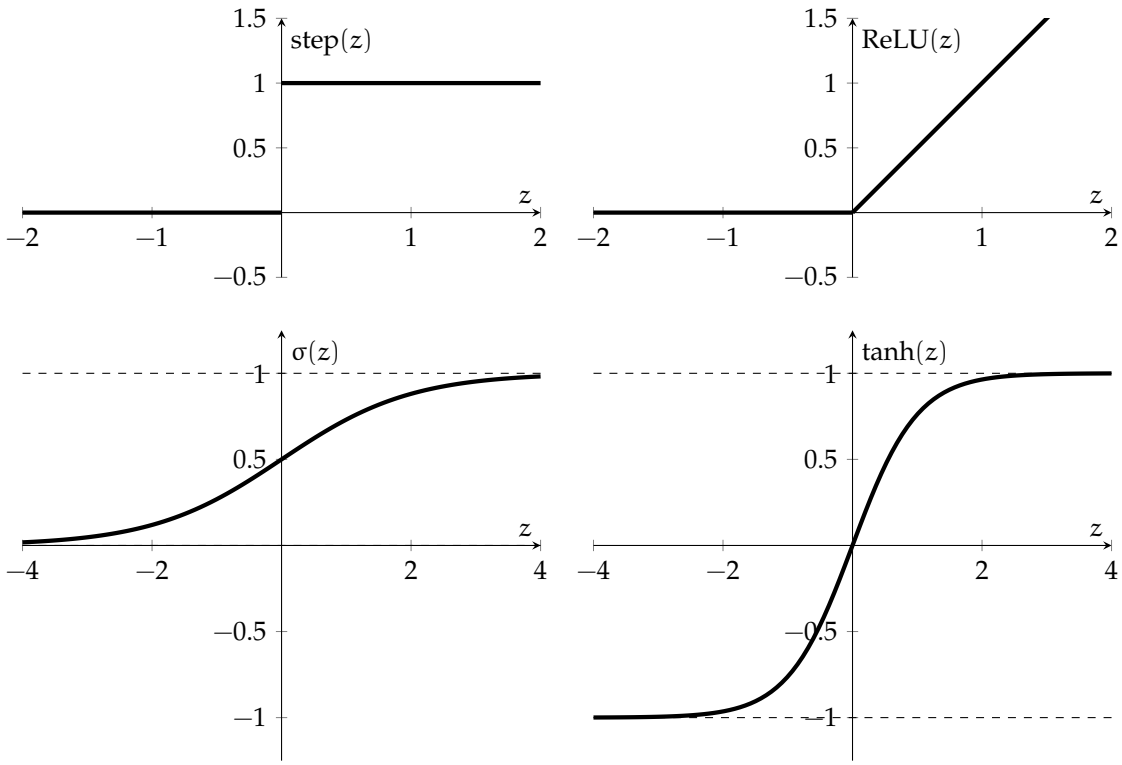
$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

Hyperbolic tangent: Always in the range $(-1, 1)$

$$\tanh(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

Softmax function: Takes a whole vector $Z \in \mathbb{R}^n$ and generates as output a vector $A \in (0, 1)^n$ with the property that $\sum_{i=1}^{n} A_i = 1$, which means we can interpret it as a probability distribution over n items:

$$\text{softmax}(z) = \begin{bmatrix} \exp(z_1) / \sum_i \exp(z_i) \\ \vdots \\ \exp(z_n) / \sum_i \exp(z_i) \end{bmatrix}$$



The original idea for neural networks involved using the **step** function as an activation, but because the derivative of the step function is zero everywhere except at the discontinuity (and there it is undefined), gradient-descent methods won't be useful in finding a good setting of the weights, and so we won't consider them further. They have been replaced, in a sense, by the sigmoid, relu, and tanh activation functions.

Study Question: Consider sigmoid, relu, and tanh activations. Which one is most like a step function? Is there an additional parameter you could add to a sigmoid that would make it be more like a step function?

Study Question: What is the derivative of the relu function? Are there some values of the input for which the derivative vanishes?

ReLUs are especially common in internal ("hidden") layers, and sigmoid activations are common for the output for binary classification and softmax for multi-class classification (see section 4 for an explanation).

4 Error back-propagation

We will train neural networks using gradient descent methods. It's possible to use *batch* gradient descent, in which we sum up the gradient over all the points (as in section 2 of chapter 6) or stochastic gradient descent (SGD), in which we take a small step with respect to the gradient considering a single point at a time (as in section 4 of chapter 6).

Our notation is going to get pretty hairy pretty quickly. To keep it as simple as we can, we'll focus on computing the contribution of one data point $x^{(i)}$ to the gradient of the loss with respect to the weights, for SGD; you can simply sum up these gradients over all the data points if you wish to do batch descent.

So, to do SGD for a training example (x, y), we need to compute $\nabla_W \text{Loss}(\text{NN}(x; W), y)$,

where W represents all weights W^l, W_0^l in all the layers $l = (1, \ldots, L)$. This seems terrifying, but is actually quite easy to do using the chain rule.

Remember the chain rule! If $a = f(b)$ and $b = g(c)$ (so that $a = f(g(c))$), then $\frac{da}{dc} = \frac{da}{db} \cdot \frac{db}{dc} = f'(b)g'(c) = f'(g(c))g'(c)$.

Remember that we are always computing the gradient of the loss function *with respect to the weights* for a particular value of (x, y). That tells us how much we want to change the weights, in order to reduce the loss incurred on this particular training example.

First, let's see how the loss depends on the weights in the final layer, W^L. Remembering that our output is A^L, and using the shorthand loss to stand for $\text{Loss}((\text{NN}(x; W), y)$ which is equal to $\text{Loss}(A^L, y)$, and finally that $A^L = f^L(Z^L)$ and $Z^L = W^{L\,T} A^{L-1} + W_0^L$, we can use the chain rule, stated informally as:

$$\frac{\partial \text{loss}}{\partial W^L} = \underbrace{\frac{\partial \text{loss}}{\partial A^L}}_{\text{depends on loss function}} \cdot \underbrace{\frac{\partial A^L}{\partial Z^L}}_{f^{L\prime}} \cdot \underbrace{\frac{\partial Z^L}{\partial W^L}}_{A^{L-1}} .$$

It might reasonably bother you that $\partial Z^L / \partial W^L = A^{L-1}$. We're somehow thinking about the derivative of a vector with respect to a matrix, which seems like it might need to be a three-dimensional thing. But note that $\partial Z^L / \partial W^L$ is really $(\partial W^{L\,T} A^{L-1}) / \partial W^L$ and it seems okay in at least an informal sense that it's A^{L-1}.

To actually get the dimensions to match, we need to write this a bit more carefully, and note that it is true for any l, including $l = L$:

$$\underbrace{\frac{\partial \text{loss}}{\partial W^l}}_{m^l \times n^l} = \underbrace{A^{l-1}}_{m^l \times 1} \underbrace{\left(\frac{\partial \text{loss}}{\partial Z^l}\right)^T}_{1 \times n^l} \tag{8.1}$$

Yay! So, in order to find the gradient of the loss with respect to the weights in the other layers of the network, we just need to be able to find $\partial \text{loss} / \partial Z^l$.

Note that we use the denominator-layout convention for matrix calculus in these notes.

If we repeatedly apply the chain rule, we get this expression for the gradient of the loss with respect to the pre-activation in the first layer, again stated informally as:

$$\frac{\partial \text{loss}}{\partial Z^1} = \underbrace{\underbrace{\frac{\partial \text{loss}}{\partial A^L} \cdot \frac{\partial A^L}{\partial Z^L} \cdot \frac{\partial Z^L}{\partial A^{L-1}} \cdot \frac{\partial A^{L-1}}{\partial Z^{L-1}} \cdot \cdots \cdot \frac{\partial A^2}{\partial Z^2}}_{\partial \text{loss} / \partial Z^2} \cdot \frac{\partial Z^2}{\partial A^1}}_{\partial \text{loss} / \partial A^1} \cdot \frac{\partial A^1}{\partial Z^1} . \tag{8.2}$$

This derivation was informal, to show you the general structure of the computation. In fact, to get the dimensions to all work out, we just have to write it backwards! Let's first understand more about these quantities:

- $\partial \text{loss} / \partial A^L$ is $n^L \times 1$ and depends on the particular loss function you are using.
- $\partial Z^l / \partial A^{l-1}$ is $m^l \times n^l$ and is just W^l (you can verify this by computing a single entry $\partial Z_i^l / \partial A_j^{l-1}$).
- $\partial A^l / \partial Z^l$ is $n^l \times n^l$. It's a little tricky to think about. Each element $a_i^l = f^l(z_i^l)$. This means that $\partial a_i^l / \partial z_j^l = 0$ whenever $i \neq j$. So, the off-diagonal elements of $\partial A^l / \partial Z^l$ are all 0, and the diagonal elements are $\partial a_i^l / \partial z_j^l = f^{l\prime}(z_j^l)$.

We are treating element-wise activation functions here; consideration of activation layers where an output a_i depends on multiple z_j, such as *softmax*, may result in a gradient matrix with non-zero off-diagonal elements.

Now, we can rewrite equation 8.2 so that the quantities match up as

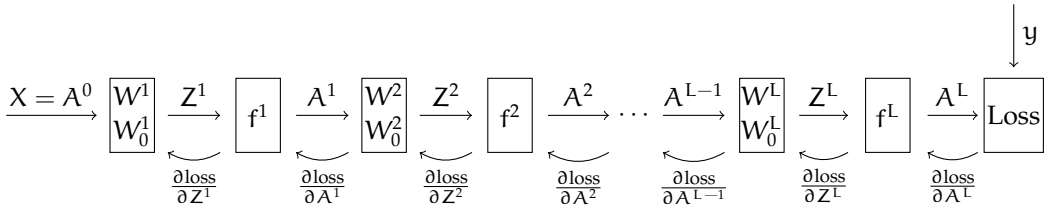
$$\frac{\partial \text{loss}}{\partial Z^l} = \frac{\partial A^l}{\partial Z^l} \cdot W^{l+1} \cdot \frac{\partial A^{l+1}}{\partial Z^{l+1}} \cdot \ldots W^{L-1} \cdot \frac{\partial A^{L-1}}{\partial Z^{L-1}} \cdot W^L \cdot \frac{\partial A^L}{\partial Z^L} \cdot \frac{\partial \text{loss}}{\partial A^L} \tag{8.3}$$

Using equation 8.3 to compute $\partial \text{loss} / \partial Z^l$ combined with equation 8.1, lets us find the gradient of the loss with respect to any of the weight matrices.

Study Question: Apply the same reasoning to find the gradients of loss with respect to W_0^l.

This general process is called *error back-propagation*. The idea is that we first do a *forward pass* to compute all the a and z values at all the layers, and finally the actual loss on this example. Then, we can work backward and compute the gradient of the loss with respect to the weights in each layer, starting at layer L and going back to layer 1.

We could call this "blame propagation". You can think of loss as how mad we are about the prediction that the network just made. Then $\partial \text{loss}/\partial A^L$ is how much we blame A^L for the loss. The last module has to take in $\partial \text{loss}/\partial A^L$ and compute $\partial \text{loss}/\partial Z^L$, which is how much we blame Z^L for the loss. The next module (working backwards) takes in $\partial \text{loss}/\partial Z^L$ and computes $\partial \text{loss}/\partial A^{L-1}$. So every module is accepting its blame for the loss, computing how much of it to allocate to each of its inputs, and passing the blame back to them.



If we view our neural network as a sequential composition of modules (in our work so far, it has been an alternation between a linear transformation with a weight matrix, and a component-wise application of a non-linear activation function), then we can define a simple API for a module that will let us compute the forward and backward passes, as well as do the necessary weight updates for gradient descent. Each module has to provide the following "methods." We are already using letters a, x, y, z with particular meanings, so here we will use u as the vector input to the module and v as the vector output:

- forward: $u \to v$
- backward: $u, v, \partial L/\partial v \to \partial L/\partial u$
- weight grad: $u, \partial L/\partial v \to \partial L/\partial W$ only needed for modules that have weights W

In homework we will ask you to implement these modules for neural network components, and then use them to construct a network and train it as described in the next section.

5 Training

Here we go! Here's how to do stochastic gradient descent training on a feed-forward neural network. After this pseudo-code, we motivate the choice of initialization in lines 2 and 3. The actual computation of the gradient values (e.g. $\partial \text{loss}/\partial A^L$) is not directly defined in this code, because we want to make the structure of the computation clear.

Study Question: What is $\partial Z^l/\partial W^l$?

Study Question: Which terms in the code below depend on f^L?

SGD-NEURAL-NET($\mathcal{D}_n, T, L, (m^1, \ldots, m^L), (f^1, \ldots, f^L)$)

for $l = 1$ **to** L
  $W^l_{ij} \sim \text{Gaussian}(0, 1/m^l)$
  $W^l_{0j} \sim \text{Gaussian}(0, 1)$
for $t = 1$ **to** T
  $i =$ random sample from $\{1, \ldots, n\}$
  $A^0 = x^{(i)}$
  // forward pass to compute the output A^L
  for $l = 1$ **to** L
    $Z^l = W^{lT} A^{l-1} + W^l_0$
    $A^l = f^l(Z^l)$
  loss $= \text{Loss}(A^L, y^{(i)})$
  for $l = L$ **to** 1:
    // error back-propagation
    $\partial \text{loss}/\partial A^l =$ **if** $l < L$ **then** $\partial \text{loss}/\partial Z^{l+1} \cdot \partial Z^{l+1}/\partial A^l$ **else** $\partial \text{loss}/\partial A^L$
    $\partial \text{loss}/\partial Z^l = \partial \text{loss}/\partial A^l \cdot \partial A^l/\partial Z^l$
    // compute gradient with respect to weights
    $\partial \text{loss}/\partial W^l = \partial \text{loss}/\partial Z^l \cdot \partial Z^l/\partial W^l$
    $\partial \text{loss}/\partial W^l_0 = \partial \text{loss}/\partial Z^l \cdot \partial Z^l/\partial W^l_0$
    // stochastic gradient descent update
    $W^l = W^l - \eta(t) \cdot \partial \text{loss}/\partial W^l$
    $W^l_0 = W^l_0 - \eta(t) \cdot \partial \text{loss}/\partial W^l_0$

Initializing W is important; if you do it badly there is a good chance the neural network training won't work well. First, it is important to initialize the weights to random values. We want different parts of the network to tend to "address" different aspects of the problem; if they all start at the same weights, the symmetry will often keep the values from moving in useful directions. Second, many of our activation functions have (near) zero slope when the pre-activation z values have large magnitude, so we generally want to keep the initial weights small so we will be in a situation where the gradients are non-zero, so that gradient descent will have some useful signal about which way to go.

One good general-purpose strategy is to choose each weight at random from a Gaussian (normal) distribution with mean 0 and standard deviation $(1/m)$ where m is the number of inputs to the unit.

Study Question: If the input x to this unit is a vector of 1's, what would the expected pre-activation z value be with these initial weights?

We write this choice (where $\sim$ means "is drawn randomly from the distribution")

$$W^l_{ij} \sim \text{Gaussian}\left(0, \frac{1}{m^l}\right) \quad .$$

It will often turn out (especially for fancier activations and loss functions) that computing

$$\frac{\partial \text{loss}}{\partial Z^L}$$

is easier than computing

$$\frac{\partial \text{loss}}{\partial A^L} \quad \text{and} \quad \frac{\partial A^L}{\partial Z^L} \quad .$$

So, we may instead ask for an implementation of a loss function to provide a backward method that computes $\partial \text{loss}/\partial Z^L$ directly.

6 Loss functions and activation functions

Different loss functions make different assumptions about the range of inputs they will get as input and, as we have seen, different activation functions will produce output values in different ranges. When you are designing a neural network, it's important to make these things fit together well. In particular, we will think about matching loss functions with the activation function in the last layer, f^L. Here is a table of loss functions and activations that make sense for them:

Loss	f^L
squared	linear
hinge	linear
NLL	sigmoid
NLLM	softmax

6.1 Two-class classification and log likelihood

For classification, the natural loss function is 0-1 loss, but we have already discussed the fact that it's very inconvenient for gradient-based learning because its derivative is discontinuous.

We have also explored *negative log likelihood* (NLL) in chapter 5. It is nice and smooth, and extends nicely to multiple classes as we will see below.

Hinge loss gives us another way, for binary classification problems, to make a smoother objective, penalizing the *margin*s of the labeled points relative to the separator. The hinge loss is defined to be

$$\mathcal{L}_h(\text{guess}, \text{actual}) = \max(1 - \text{guess} \cdot \text{actual}, 0) \ ,$$

when actual $\in \{+1, -1\}$. It has the property that, if the sign of guess is the same as the sign of actual and the magnitude of guess is greater than 1, then the loss is 0.

It is trying to enforce not only that the guess have the correct sign, but also that it should be some distance away from the separator. Using hinge loss, together with a squared-norm regularizer, actually forces the learning process to try to find a separator that has the maximum *margin* relative to the data set. This optimization set-up is called a *support vector machine*, and was popular before the renaissance of neural networks and gradient descent, because it has a quadratic form that makes it particularly easy to optimize.

6.2 Multi-class classification and log likelihood

We can extend the idea of NLL directly to multi-class classification with K classes, where the training label is represented with the one-hot vector $y = \begin{bmatrix} y_1, \ldots, y_K \end{bmatrix}^T$, where $y_k = 1$ if the example is of class k. Assume that our network uses *softmax* as the activation function in the last layer, so that the output is $a = \begin{bmatrix} a_1, \ldots, a_K \end{bmatrix}^T$, which represents a probability distribution over the K possible classes. Then, the probability that our network predicts the correct class for this example is $\prod_{k=1}^{K} a_k^{y_k}$ and the log of the probability that it is correct is $\sum_{k=1}^{K} y_k \log a_k$, so

$$\mathcal{L}_{\text{nllm}}(\text{guess}, \text{actual}) = -\sum_{k=1}^{K} \text{actual}_k \cdot \log(\text{guess}_k) \ .$$

We'll call this NLLM for *negative log likelihood multiclass.*

Study Question: Show that L_{nllm} for $K = 2$ is the same as L_{nll}.

7 Optimizing neural network parameters

Because neural networks are just parametric functions, we can optimize loss with respect to the parameters using standard gradient-descent software, but we can take advantage of the structure of the loss function and the hypothesis class to improve optimization. As we have seen, the modular function-composition structure of a neural network hypothesis makes it easy to organize the computation of the gradient. As we have also seen earlier, the structure of the loss function as a sum over terms, one per training data point, allows us to consider stochastic gradient methods. In this section we'll consider some alternative strategies for organizing training, and also for making it easier to handle the step-size parameter.

7.1 Batches

Assume that we have an objective of the form

$$J(W) = \sum_{i=1}^{n} \mathcal{L}(h(x^{(i)}; W), y^{(i)}) \ ,$$

where h is the function computed by a neural network, and W stands for all the weight matrices and vectors in the network.

When we perform *batch* gradient descent, we use the update rule

$$W := W - \eta \nabla_W J(W) \ ,$$

which is equivalent to

$$W := W - \eta \sum_{i=1}^{n} \nabla_W \mathcal{L}(h(x^{(i)}; W), y^{(i)}) \ .$$

So, we sum up the gradient of loss at each training point, with respect to W, and then take a step in the negative direction of the gradient.

In *stochastic* gradient descent, we repeatedly pick a point $(x^{(i)}, y^{(i)})$ at random from the data set, and execute a weight update on that point alone:

$$W := W - \eta \nabla_W \mathcal{L}(h(x^{(i)}; W), y^{(i)}) \ .$$

As long as we pick points uniformly at random from the data set, and decrease η at an appropriate rate, we are guaranteed, with high probability, to converge to at least a local optimum.

These two methods have offsetting virtues. The batch method takes steps in the exact gradient direction but requires a lot of computation before even a single step can be taken, especially if the data set is large. The stochastic method begins moving right away, and can sometimes make very good progress before looking at even a substantial fraction of the whole data set, but if there is a lot of variability in the data, it might require a very small η to effectively average over the individual steps moving in "competing" directions.

An effective strategy is to "average" between batch and stochastic gradient descent by using *mini-batches*. For a mini-batch of size k, we select k distinct data points uniformly at random from the data set and do the update based just on their contributions to the gradient

$$W := W - \eta \sum_{i=1}^{k} \nabla_W \mathcal{L}(h(x^{(i)}; W), y^{(i)}) \ .$$

Most neural network software packages are set up to do mini-batches.

Study Question: For what value of k is mini-batch gradient descent equivalent to stochastic gradient descent? To batch gradient descent?

Picking k unique data points at random from a large data-set is potentially computationally difficult. An alternative strategy, if you have an efficient procedure for randomly shuffling the data set (or randomly shuffling a list of indices into the data set) is to operate in a loop, roughly as follows:

MINI-BATCH-SGD(NN, data, k)

```
1  n = length(data)
2  while not done:
3      RANDOM-SHUFFLE(data)
4      for i = 1 to ⌈n/k⌉
5          BATCH-GRADIENT-UPDATE(NN, data[(i − 1)k : ik])
```

See note on the ceiling[1] function, for the case when n/k is not an integer.

7.2 Adaptive step-size

Picking a value for η is difficult and time-consuming. If it's too small, then convergence is slow and if it's too large, then we risk divergence or slow convergence due to oscillation. This problem is even more pronounced in stochastic or mini-batch mode, because we know we need to decrease the step size for the formal guarantees to hold.

It's also true that, within a single neural network, we may well want to have different step sizes. As our networks become *deep* (with increasing numbers of layers) we can find that magnitude of the gradient of the loss with respect the weights in the last layer, $\partial \text{loss}/\partial W_L$, may be substantially different from the gradient of the loss with respect to the weights in the first layer $\partial \text{loss}/\partial W_1$. If you look carefully at equation 8.3, you can see that the output gradient is multiplied by all the weight matrices of the network and is "fed back" through all the derivatives of all the activation functions. This can lead to a problem of *exploding* or *vanishing* gradients, in which the back-propagated gradient is much too big or small to be used in an update rule with the same step size.

So, we'll consider having an independent step-size parameter *for each weight*, and updating it based on a local view of how the gradient updates have been going.

This section is very strongly influenced by Sebastian Ruder's excellent blog posts on the topic: ruder.io/optimizing-gradient-descent

7.2.1 Running averages

We'll start by looking at the notion of a *running average*. It's a computational strategy for estimating a possibly weighted average of a sequence of data. Let our data sequence be $a_1, a_2, \ldots$; then we define a sequence of running average values, $A_0, A_1, A_2, \ldots$ using the equations

$$\begin{aligned} A_0 &= 0 \\ A_t &= \gamma_t A_{t-1} + (1-\gamma_t) a_t \end{aligned}$$

where $\gamma_t \in (0,1)$. If γ_t is a constant, then this is a *moving* average, in which

$$\begin{aligned} A_T &= \gamma A_{T-1} + (1-\gamma) a_T \\ &= \gamma(\gamma A_{T-2} + (1-\gamma) a_{T-1}) + (1-\gamma) a_T \\ &= \sum_{t=1}^{T} \gamma^{T-t} (1-\gamma) a_t \end{aligned}$$

[1] In line 4 of the algorithm above, $\lceil \cdot \rceil$ is known as the *ceiling* function; it returns the smallest integer greater than or equal to its input. E.g., $\lceil 2.5 \rceil = 3$ and $\lceil 3 \rceil = 3$.

So, you can see that inputs a_t closer to the end of the sequence T have more effect on A_T than early inputs.

If, instead, we set $\gamma_t = (t-1)/t$, then we get the actual average.

Study Question: Prove to yourself that the previous assertion holds.

7.2.2 Momentum

Now, we can use methods that are a bit like running averages to describe strategies for computing η. The simplest method is *momentum*, in which we try to "average" recent gradient updates, so that if they have been bouncing back and forth in some direction, we take out that component of the motion. For momentum, we have

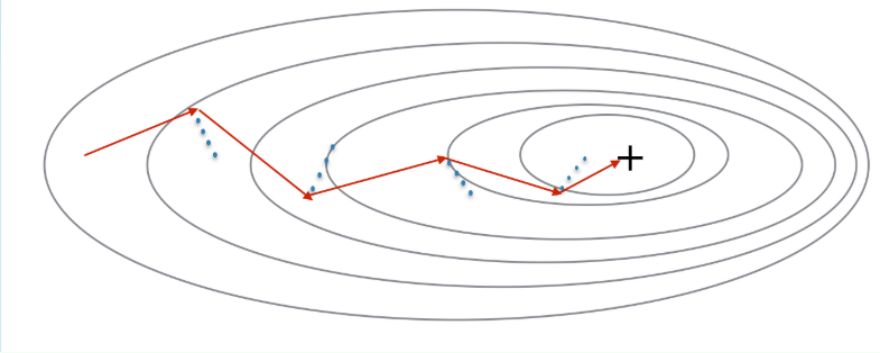
$$\begin{aligned} V_0 &= 0 \\ V_t &= \gamma V_{t-1} + \eta \nabla_W J(W_{t-1}) \\ W_t &= W_{t-1} - V_t \end{aligned}$$

This doesn't quite look like an adaptive step size. But what we can see is that, if we let $\eta = \eta'(1-\gamma)$, then the rule looks exactly like doing an update with step size η' on a moving average of the gradients with parameter γ:

$$\begin{aligned} M_0 &= 0 \\ M_t &= \gamma M_{t-1} + (1-\gamma)\nabla_W J(W_{t-1}) \\ W_t &= W_{t-1} - \eta' M_t \end{aligned}$$

Study Question: Prove to yourself that these formulations are equivalent.

We will find that V_t will be bigger in dimensions that consistently have the same sign for ∇_W and smaller for those that don't. Of course we now have *two* parameters to set (η and γ), but the hope is that the algorithm will perform better overall, so it will be worth trying to find good values for them. Often γ is set to be something like 0.9.



The red arrows show the update after one step of mini-batch gradient descent with momentum. The blue points show the direction of the gradient with respect to the mini-batch at each step. Momentum smooths the path taken towards the local minimum and leads to faster convergence.

Study Question: If you set $\gamma = 0.1$, would momentum have more of an effect or less of an effect than if you set it to 0.9?

7.2.3 Adadelta

Another useful idea is this: we would like to take larger steps in parts of the space where $J(W)$ is nearly flat (because there's no risk of taking too big a step due to the gradient being large) and smaller steps when it is steep. We'll apply this idea to each weight independently, and end up with a method called *adadelta*, which is a variant on *adagrad* (for adaptive gradient). Even though our weights are indexed by layer, input unit and output unit, for simplicity here, just let W_j be any weight in the network (we will do the same thing for all of them).

$$\begin{aligned} g_{t,j} &= \nabla_W J(W_{t-1})_j \\ G_{t,j} &= \gamma G_{t-1,j} + (1-\gamma) g_{t,j}^2 \\ W_{t,j} &= W_{t-1,j} - \frac{\eta}{\sqrt{G_{t,j} + \epsilon}} g_{t,j} \end{aligned}$$

The sequence $G_{t,j}$ is a moving average of the square of the jth component of the gradient. We square it in order to be insensitive to the sign—we want to know whether the magnitude is big or small. Then, we perform a gradient update to weight j, but divide the step size by $\sqrt{G_{t,j} + \epsilon}$, which is larger when the surface is steeper in direction j at point W_{t-1} in weight space; this means that the step size will be smaller when it's steep and larger when it's flat.

7.2.4 Adam

Adam has become the default method of managing step sizes in neural networks. It combines the ideas of momentum and adadelta. We start by writing moving averages of the gradient and squared gradient, which reflect estimates of the mean and variance of the gradient for weight j:

Although, interestingly, it may actually violate the convergence conditions of SGD: arxiv.org/abs/1705.08292

$$\begin{aligned} g_{t,j} &= \nabla_W J(W_{t-1})_j \\ m_{t,j} &= B_1 m_{t-1,j} + (1-B_1) g_{t,j} \\ v_{t,j} &= B_2 v_{t-1,j} + (1-B_2) g_{t,j}^2 \quad . \end{aligned}$$

A problem with these estimates is that, if we initialize $m_0 = v_0 = 0$, they will always be biased (slightly too small). So we will correct for that bias by defining

$$\begin{aligned} \hat{m}_{t,j} &= \frac{m_{t,j}}{1 - B_1^t} \\ \hat{v}_{t,j} &= \frac{v_{t,j}}{1 - B_2^t} \\ W_{t,j} &= W_{t-1,j} - \frac{\eta}{\sqrt{\hat{v}_{t,j} + \epsilon}} \hat{m}_{t,j} \quad . \end{aligned}$$

Note that B_1^t is B_1 raised to the power t, and likewise for B_2^t. To justify these corrections, note that if we were to expand $m_{t,j}$ in terms of $m_{0,j}$ and $g_{0,j}, g_{1,j}, \ldots, g_{t,j}$ the coefficients would sum to 1. However, the coefficient behind $m_{0,j}$ is B_1^t and since $m_{0,j} = 0$, the sum of coefficients of non-zero terms is $1 - B_1^t$, hence the correction. The same justification holds for $v_{t,j}$.

Now, our update for weight j has a step size that takes the steepness into account, as in adadelta, but also tends to move in the same direction, as in momentum. The authors of this method propose setting $B_1 = 0.9, B_2 = 0.999, \epsilon = 10^{-8}$. Although we now have even more parameters, Adam is not highly sensitive to their values (small changes do not have a huge effect on the result).

Study Question: Define $\hat{m}_j$ directly as a moving average of $g_{t,j}$. What is the decay (γ parameter)?

Even though we now have a step-size for each weight, and we have to update various quantities on each iteration of gradient descent, it's relatively easy to implement by maintaining a matrix for each quantity ($m_t^\ell, v_t^\ell, g_t^\ell, {g_t^2}^\ell$) in each layer of the network.

8 Regularization

So far, we have only considered optimizing loss on the training data as our objective for neural network training. But, as we have discussed before, there is a risk of overfitting if we do this. The pragmatic fact is that, in current deep neural networks, which tend to be very large and to be trained with a large amount of data, overfitting is not a huge problem. This runs counter to our current theoretical understanding and the study of this question is a hot area of research. Nonetheless, there are several strategies for regularizing a neural network, and they can sometimes be important.

8.1 Methods related to ridge regression

One group of strategies can, interestingly, be shown to have similar effects: early stopping, weight decay, and adding noise to the training data.

Result is due to Bishop, described in his textbook and here doi.org/10.1162/neco.1995.7.1.108.

Early stopping is the easiest to implement and is in fairly common use. The idea is to train on your training set, but at every *epoch* (pass through the whole training set, or possibly more frequently), evaluate the loss of the current W on a *validation set*. It will generally be the case that the loss on the training set goes down fairly consistently with each iteration, the loss on the validation set will initially decrease, but then begin to increase again. Once you see that the validation loss is systematically increasing, you can stop training and return the weights that had the lowest validation error.

Another common strategy is to simply penalize the norm of all the weights, as we did in ridge regression. This method is known as *weight decay*, because when we take the gradient of the objective

$$J(W) = \sum_{i=1}^{n} \text{Loss}(\text{NN}(x^{(i)}), y^{(i)}; W) + \lambda \|W\|^2$$

we end up with an update of the form

$$\begin{aligned} W_t &= W_{t-1} - \eta \left(\left(\nabla_W \text{Loss}(\text{NN}(x^{(i)}), y^{(i)}; W_{t-1}) \right) + 2\lambda W_{t-1} \right) \\ &= W_{t-1}(1 - 2\lambda\eta) - \eta \left(\nabla_W \text{Loss}(\text{NN}(x^{(i)}), y^{(i)}; W_{t-1}) \right) \quad . \end{aligned}$$

This rule has the form of first "decaying" W_{t-1} by a factor of $(1 - 2\lambda\eta)$ and then taking a gradient step.

Finally, the same effect can be achieved by perturbing the $x^{(i)}$ values of the training data by adding a small amount of zero-mean normally distributed noise before each gradient computation. It makes intuitive sense that it would be more difficult for the network to overfit to particular training data if they are changed slightly on each training step.

8.2 Dropout

Dropout is a regularization method that was designed to work with deep neural networks. The idea behind it is, rather than perturbing the data every time we train, we'll perturb the network! We'll do this by randomly, on each training step, selecting a set of units in each

layer and prohibiting them from participating. Thus, all of the units will have to take a kind of "collective" responsibility for getting the answer right, and will not be able to rely on any small subset of the weights to do all the necessary computation. This tends also to make the network more robust to data perturbations.

During the training phase, for each training example, for each unit, randomly with probability p temporarily set $a_j^\ell := 0$. There will be no contribution to the output and no gradient update for the associated unit.

Study Question: Be sure you understand why, when using SGD, setting an activation value to 0 will cause that unit's weights not to be updated on that iteration.

When we are done training and want to use the network to make predictions, we multiply all weights by p to achieve the same average activation levels.

Implementing dropout is easy! In the forward pass during training, we let

$$a^\ell = f(z^\ell) * d^\ell$$

where $*$ denotes component-wise product and d^ℓ is a vector of 0's and 1's drawn randomly with probability p. The backwards pass depends on a^ℓ, so we do not need to make any further changes to the algorithm.

It is common to set p to 0.5, but this is something one might experiment with to get good results on your problem and data.

8.3 Batch Normalization

A more modern alternative to dropout, which tends to achieve better performance, is *batch normalization*. It was originally developed to address a problem of *covariate shift*: that is, if you consider the second layer of a two-layer neural network, the distribution of its input values is changing over time as the first layer's weights change. Learning when the input distribution is changing is extra difficult: you have to change your weights to improve your predictions, but also just to compensate for a change in your inputs (imagine, for instance, that the magnitude of the inputs to your layer is increasing over time—then your weights will have to decrease, just to keep your predictions the same).

For more details see `arxiv.org/abs/1502.03167`.

So, when training with mini-batches, the idea is to *standardize* the input values for each mini-batch, just in the way that we did it in section 2.3 of chapter 4, subtracting off the mean and dividing by the standard deviation of each input dimension. This means that the scale of the inputs to each layer remains the same, no matter how the weights in previous layers change. However, this somewhat complicates matters, because the computation of the weight updates will need to take into account that we are performing this transformation. In the modular view, batch normalization can be seen as a module that is applied to z^l, interposed after the product with W^l and before input to f^l.

Batch normalization ends up having a regularizing effect for similar reasons that adding noise and dropout do: each mini-batch of data ends up being mildly perturbed, which prevents the network from exploiting very particular values of the data points.

We follow here the suggestion from the original paper of applying batch normalization before the activation function. Since then it has been shown that, in some cases, applying it after works a bit better. But there isn't any definite findings on which works better and when.

Let's think of the batch-norm layer as taking z^l as input and producing an output $\widehat{Z}^l$ as output. But now, instead of thinking of Z^l as an $n^l \times 1$ vector, we have to explicitly think about handling a mini-batch of data of size K, all at once, so Z^l will be $n^l \times K$, and so will the output $\widehat{Z}^l$.

Our first step will be to compute the *batchwise* mean and standard deviation. Let μ^l be the $n^l \times 1$ vector where

$$\mu_i^l = \frac{1}{K} \sum_{j=1}^{K} Z_{ij}^l \ ,$$

and let σ^l be the $n^l \times 1$ vector where

$$\sigma_i^l = \sqrt{\frac{1}{K}\sum_{j=1}^{K}(Z_{ij}^l - \mu_i)^2} \ .$$

The basic normalized version of our data would be a matrix, element (i,j) of which is

$$\overline{Z}_{ij}^l = \frac{Z_{ij}^l - \mu_i^l}{\sigma_i^l + \epsilon} \ ,$$

where ϵ is a very small constant to guard against division by zero. However, if we let these be our $\widehat{Z}^l$ values, we really are forcing something too strong on our data—our goal was to normalize across the data batch, but not necessarily force the output values to have exactly mean 0 and standard deviation 1. So, we will give the layer the "opportunity" to shift and scale the outputs by adding new weights to the layer. These weights are G^l and B^l, each of which is an $n^l \times 1$ vector. Using the weights, we define the final output to be

$$\widehat{Z}_{ij}^l = G_i^l \overline{Z}_{ij}^l + B_i^l \ .$$

That's the forward pass. Whew!

Now, for the backward pass, we have to do two things: given $\partial L/\partial \widehat{Z}^l$,

- Compute $\partial L/\partial Z^l$ for back-propagation, and
- Compute $\partial L/\partial G^l$ and $\partial L/\partial B^l$ for gradient updates of the weights in this layer.

Schematically

$$\frac{\partial L}{\partial B} = \frac{\partial L}{\partial \widehat{Z}}\frac{\partial \widehat{Z}}{\partial B} \ .$$

For simplicity we will drop the reference to the layer l in the rest of the derivation

It's hard to think about these derivatives in matrix terms, so we'll see how it works for the components. B_i contributes to $\widehat{Z}_{ij}$ for all data points j in the batch. So

$$\begin{aligned}\frac{\partial L}{\partial B_i} &= \sum_j \frac{\partial L}{\partial \widehat{Z}_{ij}}\frac{\partial \widehat{Z}_{ij}}{\partial B_i} \\ &= \sum_j \frac{\partial L}{\partial \widehat{Z}_{ij}} \ ,\end{aligned}$$

Similarly, G_i contributes to $\widehat{Z}_{ij}$ for all data points j in the batch. So

$$\begin{aligned}\frac{\partial L}{\partial G_i} &= \sum_j \frac{\partial L}{\partial \widehat{Z}_{ij}}\frac{\partial \widehat{Z}_{ij}}{\partial G_i} \\ &= \sum_j \frac{\partial L}{\partial \widehat{Z}_{ij}}\overline{Z}_{ij} \ .\end{aligned}$$

Now, let's figure out how to do backprop. We can start schematically:

$$\frac{\partial L}{\partial Z} = \frac{\partial L}{\partial \widehat{Z}}\frac{\partial \widehat{Z}}{\partial Z} \ .$$

And because dependencies only exist across the batch, but not across the unit outputs,

$$\frac{\partial L}{\partial Z_{ij}} = \sum_{k=1}^{K}\frac{\partial L}{\partial \widehat{Z}_{ik}}\frac{\partial \widehat{Z}_{ik}}{\partial Z_{ij}} \ .$$

The next step is to note that

$$\begin{aligned}\frac{\partial \widehat{Z}_{ik}}{\partial Z_{ij}} &= \frac{\partial \widehat{Z}_{ik}}{\partial \overline{Z}_{ik}} \frac{\partial \overline{Z}_{ik}}{\partial Z_{ij}} \\ &= G_i \frac{\partial \overline{Z}_{ik}}{\partial Z_{ij}}\end{aligned}$$

And now that

$$\frac{\partial \overline{Z}_{ik}}{\partial Z_{ij}} = \left(\delta_{jk} - \frac{\partial \mu_i}{\partial Z_{ij}}\right) \frac{1}{\sigma_i} - \frac{Z_{ik} - \mu_i}{\sigma_i^2} \frac{\partial \sigma_i}{\partial Z_{ij}} \quad ,$$

where $\delta_{jk} = 1$ if $j = k$ and $\delta_{jk} = 0$ otherwise. Getting close! We need two more small parts:

$$\begin{aligned}\frac{\partial \mu_i}{\partial Z_{ij}} &= \frac{1}{K} \\ \frac{\partial \sigma_i}{\partial Z_{ij}} &= \frac{Z_{ij} - \mu_i}{K\sigma_i}\end{aligned}$$

Putting the whole crazy thing together, we get

$$\frac{\partial L}{\partial Z_{ij}} = \sum_{k=1}^{K} \frac{\partial L}{\partial \widehat{Z}_{ik}} G_i \frac{1}{K\sigma_i} \left(\delta_{jk} K - 1 - \frac{(Z_{ik} - \mu_i)(Z_{ij} - \mu_i)}{\sigma_i^2}\right)$$

CHAPTER 9

Convolutional Neural Networks

So far, we have studied what are called *fully connected* neural networks, in which all of the units at one layer are connected to all of the units in the next layer. This is a good arrangement when we don't know anything about what kind of mapping from inputs to outputs we will be asking the network to learn to approximate. But if we *do* know something about our problem, it is better to build it into the structure of our neural network. Doing so can save computation time and significantly diminish the amount of training data required to arrive at a solution that generalizes robustly.

One very important application domain of neural networks, where the methods have achieved an enormous amount of success in recent years, is signal processing. Signals might be spatial (in two-dimensional camera images or three-dimensional depth or CAT scans) or temporal (speech or music). If we know that we are addressing a signal-processing problem, we can take advantage of *invariant* properties of that problem. In this chapter, we will focus on two-dimensional spatial problems (images) but use one-dimensional ones as a simple example. Later, we will address temporal problems.

Imagine that you are given the problem of designing and training a neural network that takes an image as input, and outputs a classification, which is positive if the image contains a cat and negative if it does not. An image is described as a two-dimensional array of *pixels*, each of which may be represented by three integer values, encoding intensity levels in red, green, and blue color channels.

A *pixel* is a "picture element."

There are two important pieces of prior structural knowledge we can bring to bear on this problem:

- **Spatial locality:** The set of pixels we will have to take into consideration to find a cat will be near one another in the image.
- **Translation invariance:** The pattern of pixels that characterizes a cat is the same no matter where in the image the cat occurs.

So, for example, we won't have to consider some combination of pixels in the four corners of the image, in order to see if they encode cat-ness.

Cats don't look different if they're on the left or the right side of the image.

We will design neural network structures that take advantage of these properties.

1 Filters

We begin by discussing *image filters*. An image filter is a function that takes in a local spatial neighborhood of pixel values and detects the presence of some pattern in that data.

Unfortunately in AI/ML/CS/Math, the word "filter" gets used in many ways: in addition to the one we describe here, it can describe a temporal process (in fact, our moving averages are a kind of filter) and even a somewhat esoteric algebraic structure.

Let's consider a very simple case to start, in which we have a 1-dimensional binary "image" and a filter F of size two. The filter is a vector of two numbers, which we will move along the image, taking the dot product between the filter values and the image values at each step, and aggregating the outputs to produce a new image.

Let X be the original image, of size d; then pixel i of the the output image is specified by

$$Y_i = F \cdot (X_{i-1}, X_i) \ .$$

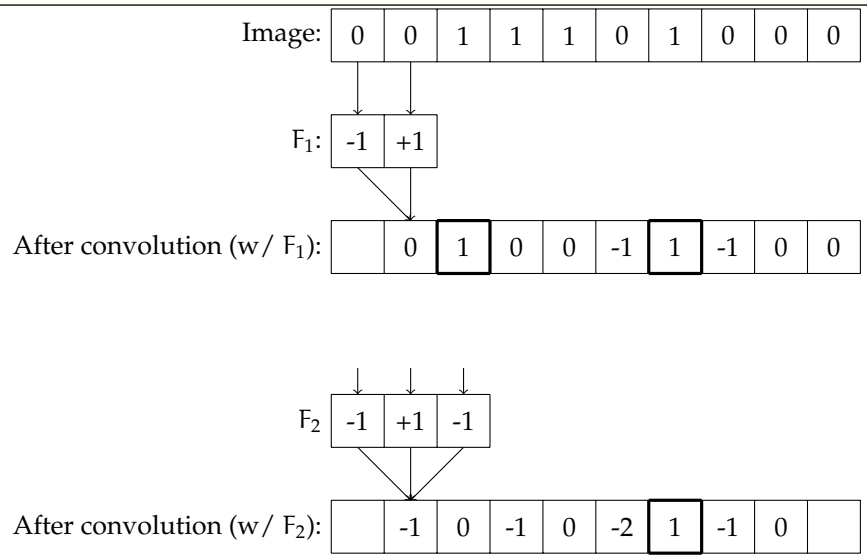
To ensure that the output image is also of dimension d, we will generally "pad" the input image with 0 values if we need to access pixels that are beyond the bounds of the input image. This process of applying the filter to the image to create a new image is called "convolution."

And filters are also sometimes called *convolutional kernels*.

If you are already familiar with what a convolution is, you might notice that this definition corresponds to what is often called a correlation and not to a convolution. Indeed, correlation and convolution refer to different operations in signal processing. However, in the neural networks literature, most libraries implement the correlation (as described in this chapter) but call it convolution. The distinction is not significant; in principle, if convolution is required to solve the problem, the network could learn the necessary weights. For a discussion of the difference between convolution and correlation and the conventions used in the literature you can read section 9.1 in this excellent book: `https://www.deeplearningbook.org`.

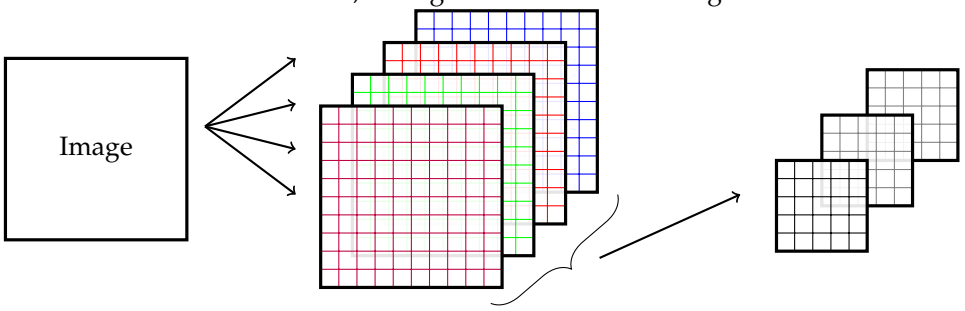
Here is a concrete example. Let the filter $F_1 = (-1, +1)$. Then given the first image below, we can convolve it with filter F_1 to obtain the second image. You can think of this filter as a detector for "left edges" in the original image—to see this, look at the places where there is a 1 in the output image, and see what pattern exists at that position in the input image. Another interesting filter is $F_2 = (-1, +1, -1)$. The third image below shows the result of convolving the first image with F_2.

Study Question: Convince yourself that filter F_2 can be understood as a detector for isolated positive pixels in the binary image.



Two-dimensional versions of filters like these are thought to be found in the visual cortex of all mammalian brains. Similar patterns arise from statistical analysis of natural

images. Computer vision people used to spend a lot of time hand-designing *filter banks*. A filter bank is a set of sets of filters, arranged as shown in the diagram below.



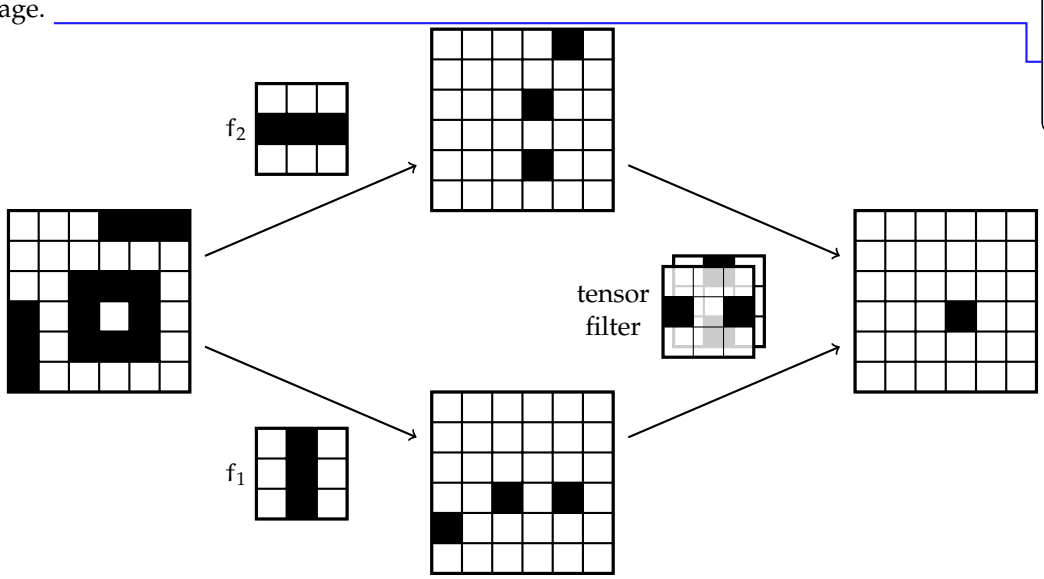
All of the filters in the first group are applied to the original image; if there are k such filters, then the result is k new images, which are called *channels*. Now imagine stacking all these new images up so that we have a cube of data, indexed by the original row and column indices of the image, as well as by the channel. The next set of filters in the filter bank will generally be *three-dimensional*: each one will be applied to a sub-range of the row and column indices of the image and to all of the channels.

These 3D chunks of data are called *tensors*. The algebra of tensors is fun, and a lot like matrix algebra, but we won't go into it in any detail.

There is a popular piece of neural-network software called *Tensorflow* that makes operations on tensors easy.

Here is a more complex example of two-dimensional filtering. We have two 3×3 filters in the first layer, f_1 and f_2. You can think of each one as "looking" for three pixels in a row, f_1 vertically and f_2 horizontally. Assuming our input image is $n \times n$, then the result of filtering with these two filters is an $n \times n \times 2$ tensor. Now we apply a tensor filter (hard to draw!) that "looks for" a combination of two horizontal and two vertical bars (now represented by individual pixels in the two channels), resulting in a single final $n \times n$ image.

When we have a color image as input, we treat it as having 3 channels, and hence as an $n \times n \times 3$ tensor.



We are going to design neural networks that have this structure. Each "bank" of the filter bank will correspond to a neural-network layer. The numbers in the individual filters will be the "weights" (plus a single additive bias or offset value for each filter) of the network, which we will train using gradient descent. What makes this interesting and powerful (and somewhat confusing at first) is that the same weights are used many many times in the computation of each layer. This *weight sharing* means that we can express a transformation on a large image with relatively few parameters; it also means we'll have to take care in figuring out exactly how to train it!

We will define a filter layer l formally with:

- *number* of filters m^l;
- *size* of one filter is $k^l \times k^l \times m^{l-1}$ plus 1 bias value (for this one filter);
- *stride* s^l is the spacing at which we apply the filter to the image; in all of our examples so far, we have used a stride of 1, but if we were to "skip" and apply the filter only at odd-numbered indices of the image, then it would have a stride of two (and produce a resulting image of half the size);
- *input tensor size* $n^{l-1} \times n^{l-1} \times m^{l-1}$
- *padding*: p^l is how many extra pixels – typically with value 0 – we add around the edges of the input. For an input of size $n^{l-1} \times n^{l-1} \times m^{l-1}$, our new effective input size with padding becomes $(n^{l-1} + 2 * p^l) \times (n^{l-1} + 2 * p^l) \times m^{l-1}$.

For simplicity, we are assuming that all images and filters are square (having the same number of rows and columns). That is in no way necessary, but is usually fine and definitely simplifies our notation.

This layer will produce an output tensor of size $n^l \times n^l \times m^l$, where $n^l = \lceil (n^{l-1} + 2 * p^l - (k^l - 1))/s^l \rceil$.[1] The weights are the values defining the filter: there will be m^l different $k^l \times k^l \times m^{l-1}$ tensors of weight values; plus each filter may have a bias term, which means there is one more weight value per filter. A filter with a bias operates just like the filter examples above, except we add the bias to the output. For instance, if we incorporated a bias term of 0.5 into the filter F_2 above, the output would be $(-0.5, 0.5, -0.5, 0.5, -1.5, 1.5, -0.5, 0.5)$ instead of $(-1, 0, -1, 0, -2, 1, -1, 0)$.

This may seem complicated, but we get a rich class of mappings that exploit image structure and have many fewer weights than a fully connected layer would.

Study Question: How many weights are in a convolutional layer specified as above?

Study Question: If we used a fully-connected layer with the same size inputs and outputs, how many weights would it have?

2 Max Pooling

It is typical to structure filter banks into a *pyramid*, in which the image sizes get smaller in successive layers of processing. The idea is that we find local patterns, like bits of edges in the early layers, and then look for patterns in those patterns, etc. This means that, effectively, we are looking for patterns in larger pieces of the image as we apply successive filters. Having a stride greater than one makes the images smaller, but does not necessarily aggregate information over that spatial range.

Both in engineering and in nature

Another common layer type, which accomplishes this aggregation, is *max pooling*. A max pooling layer operates like a filter, but has no weights. *You can think of it as a pure functional layer, like a ReLU layer in a fully connected network.* It has a filter size, as in a filter layer, but simply returns the maximum value in its field. Usually, we apply max pooling with the following traits:

We sometimes use the term *receptive field* or just *field* to mean the area of an input image that a filter is being applied to.

- stride > 1, so that the resulting image is smaller than the input image; and
- $k \geqslant$ stride, so that the whole image is covered.

[1] Recall that $\lceil \cdot \rceil$ is the *ceiling* function; it returns the smallest integer greater than or equal to its input. E.g., $\lceil 2.5 \rceil = 3$ and $\lceil 3 \rceil = 3$.

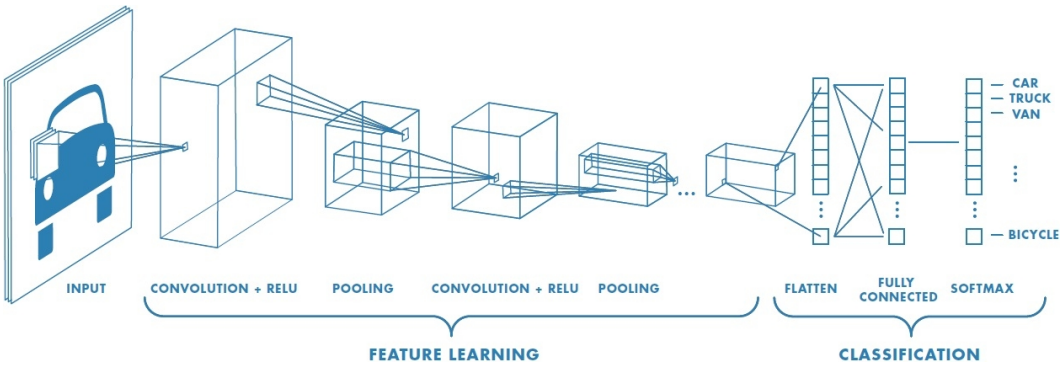
As a result of applying a max pooling layer, we don't keep track of the precise location of a pattern. This helps our filters to learn to recognize patterns independent of their location.

Consider a max pooling layer of stride $= k = 2$. This would map a $64 \times 64 \times 3$ image to a $32 \times 32 \times 3$ image. Note that max pooling layers do not have additional bias or offset values.

Study Question: Maximilian Poole thinks it would be a good idea to add two max pooling layers of size k, one right after the other, to their network. What single layer would be equivalent?

3 Typical architecture

Here is the form of a typical convolutional network:



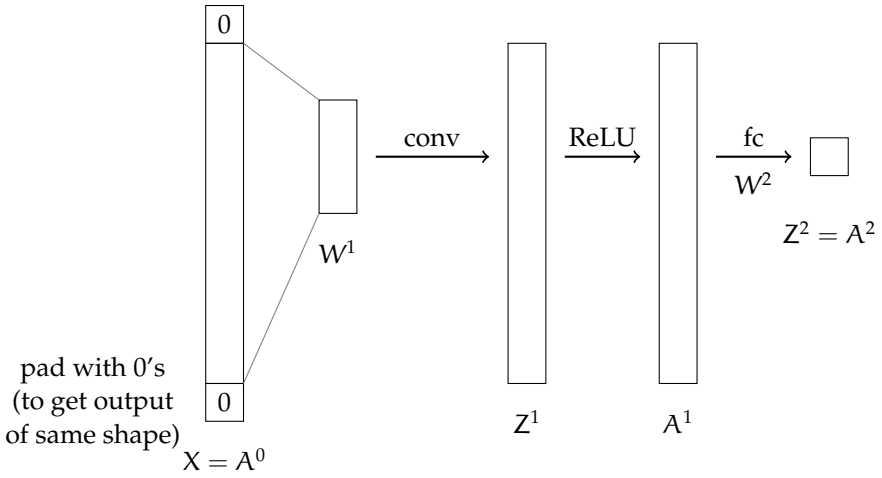
Source: https://www.mathworks.com/solutions/deep-learning/convolutional-neural-network.html

After each filter layer there is generally a ReLU layer; there maybe be multiple filter/ReLU layers, then a max pooling layer, then some more filter/ReLU layers, then max pooling. Once the output is down to a relatively small size, there is typically a last fully-connected layer, leading into an activation function such as softmax that produces the final output. The exact design of these structures is an art—there is not currently any clear theoretical (or even systematic empirical) understanding of how these various design choices affect overall performance of the network.

The critical point for us is that this is all just a big neural network, which takes an input and computes an output. The mapping is a differentiable function of the weights, which means we can adjust the weights to decrease the loss by performing gradient descent, and we can compute the relevant gradients using back-propagation!

Well, the derivative is not continuous, both because of the ReLU and the max pooling operations, but we ignore that fact.

Let's work through a *very* simple example of how back-propagation can work on a convolutional network. The architecture is shown below. Assume we have a one-dimensional single-channel image, of size $n \times 1 \times 1$ and a single $k \times 1 \times 1$ filter (where we omit the filter bias) in the first convolutional layer, denoted "conv" in the figure below. Then we pass it through a ReLU layer, and finally through a fully-connected layer, denoted "fc" below, with no additional activation function on the output.



For simplicity assume k is odd, let the input image $X = A^0$, and assume we are using squared loss. Then we can describe the forward pass as follows:

$$\begin{aligned} Z^1_i &= {W^1}^T \cdot A^0_{[i-\lfloor k/2 \rfloor : i+\lfloor k/2 \rfloor]} \\ A^1 &= \mathtt{ReLU}(Z^1) \\ A^2 = Z^2 &= {W^2}^T A^1 \\ L(A^2, y) &= (A^2 - y)^2 \end{aligned}$$

Study Question: For a filter of size k, how much padding do we need to add to the top and bottom of the image?

How do we update the weights in filter W^1?

$$\frac{\partial \text{loss}}{\partial W^1} = \frac{\partial Z^1}{\partial W^1} \cdot \frac{\partial A^1}{\partial Z^1} \cdot \frac{\partial \text{loss}}{\partial A^1}$$

- $\partial Z^1 / \partial W^1$ is the $k \times n$ matrix such that $\partial Z^1_i / \partial W^1_j = X_{i-\lfloor k/2 \rfloor + j - 1}$. So, for example, if $i = 10$, which corresponds to column 10 in this matrix, which illustrates the dependence of pixel 10 of the output image on the weights, and if $k = 5$, then the elements in column 10 will be $X_8, X_9, X_{10}, X_{11}, X_{12}$.
- $\partial A^1 / \partial Z^1$ is the $n \times n$ diagonal matrix such that

$$\partial A^1_i / \partial Z^1_i = \begin{cases} 1 & \text{if } Z^1_i > 0 \\ 0 & \text{otherwise} \end{cases}$$

- $\partial \text{loss} / \partial A^1 = \partial \text{loss} / \partial A^2 \cdot \partial A^2 / \partial A^1 = 2(A^2 - y) W^2$, an $n \times 1$ vector

Multiplying these components yields the desired gradient, of shape $k \times 1$.

CHAPTER 10

Sequential models

So far, we have limited our attention to domains in which each output y is assumed to have been generated as a function of an associated input x, and our hypotheses have been "pure" functions, in which the output depends only on the input (and the parameters we have learned that govern the function's behavior). In the next few weeks, we are going to consider cases in which our models need to go beyond functions.

- In *recurrent neural networks*, the hypothesis that we learn is not a function of a single input, but of the whole sequence of inputs that the predictor has received.
- In *reinforcement learning*, the hypothesis is either a *model* of a domain (such as a game) as a recurrent system or a *policy* which is a pure function, but whose loss is determined by the ways in which the policy interacts with the domain over time.

Before we engage with those forms of learning, we will study models of sequential or recurrent systems that underlie the learning methods.

1 State machines

A *state machine* is a description of a process (computational, physical, economic) in terms of its potential sequences of *states*.

The *state* of a system is defined to be all you would need to know about the system to predict its future trajectories as well as possible. It could be the position and velocity of an object or the locations of your pieces on a game board, or the current traffic densities on a highway network.

Formally, we define a *state machine* as $(\mathcal{S}, \mathcal{X}, \mathcal{Y}, s_0, f, g)$ where

- $\mathcal{S}$ is a finite or infinite set of possible states;
- $\mathcal{X}$ is a finite or infinite set of possible inputs;
- $\mathcal{Y}$ is a finite or infinite set of possible outputs;
- $s_0 \in \mathcal{S}$ is the initial state of the machine;
- $f : \mathcal{S} \times \mathcal{X} \to \mathcal{S}$ is a *transition function*, which takes an input and a previous state and produces a next state;

This is such a pervasive idea that it has been given many names in many subareas of computer science, control theory, physics, etc., including: *automaton*, *transducer*, *dynamical system*, *system*, etc.

There are a huge number of major and minor variations on the idea of a state machine. We'll just work with one specific one in this section and another one in the next, but don't worry if you see other variations out in the world!

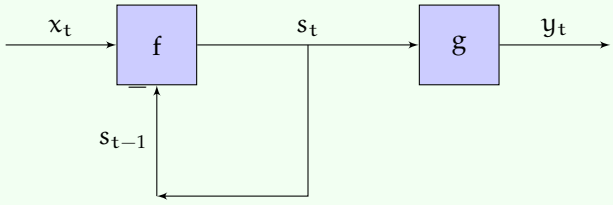
- $g : \mathcal{S} \to \mathcal{Y}$ is an *output function*, which takes a state and produces an output.

The basic operation of the state machine is to start with state s_0, then iteratively compute for $t \geqslant 1$:

In some cases, we will pick a starting state from a set or distribution.

$$s_t = f(s_{t-1}, x_t)$$
$$y_t = g(s_t)$$

The diagram below illustrates this process. Note that the "feedback" connection of s_t back into f has to be buffered or delayed by one time step—otherwise what it is computing would not generally be well defined.



So, given a sequence of inputs $x_1, x_2, \ldots$ the machine generates a sequence of outputs

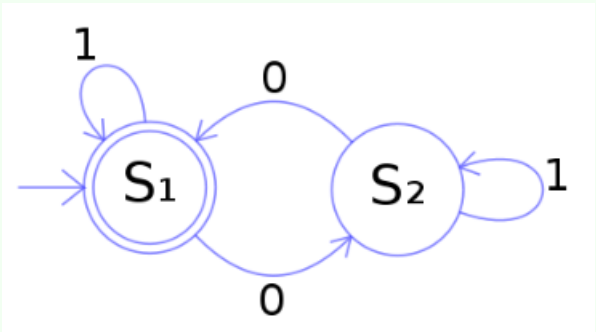
$$\underbrace{g(f(s_0, x_1))}_{y_1}, \underbrace{g(f(f(s_0, x_1), x_2))}_{y_2}, \ldots \quad .$$

We sometimes say that the machine *transduces* sequence x into sequence y. The output at time t can have dependence on inputs from steps 1 to t.

One common form is *finite state machines*, in which $\mathcal{S}$, $\mathcal{X}$, and $\mathcal{Y}$ are all finite sets. They are often described using *state transition diagrams* such as the one below, in which nodes stand for states and arcs indicate transitions. Nodes are labeled by which output they generate and arcs are labeled by which input causes the transition.

All computers can be described, at the digital level, as finite state machines. Big, but finite!

One can verify that the state machine below reads binary strings and determines the parity of the number of zeros in the given string. Check for yourself that all inputted binary strings end in state S_1 if and only if they contain an even number of zeros.



Another common structure that is simple but powerful and used in signal processing and control is *linear time-invariant (LTI) systems*. In this case, $\mathcal{S} = \mathbb{R}^m$, $\mathcal{X} = \mathbb{R}^l$ and $\mathcal{Y} = \mathbb{R}^n$, and f and g are linear functions of their inputs. In discrete time, they can be defined by a linear difference equation, like

$$y[t] = 3y[t-1] + 6y[t-2] + 5x[t] + 3x[t-2] \quad ,$$

(where $y[t]$ is y at time t) and can be implemented using state to store relevant previous input and output information.

We will study *recurrent neural networks* which are a lot like a non-linear version of an LTI system, with transition and output functions

$$f(s, x) = f_1(W^{sx}x + W^{ss}s + W_0^{ss})$$
$$g(s) = f_2(W^0 s + W_0^0)$$

defined by weight matrices

$$W^{sx} : m \times \ell$$
$$W^{ss} : m \times m$$
$$W_0^{ss} : m \times 1$$
$$W^0 : n \times m$$
$$W_0^0 : n \times 1$$

and activation functions f_1 and f_2. We will see that it's actually possible to learn weight values for a recurrent neural network using gradient descent.

2 Markov decision processes

A *Markov decision process* (MDP) is a variation on a state machine in which:

- The transition function is *stochastic*, meaning that it defines a probability distribution over the next state given the previous state and input, but each time it is evaluated it draws a new state from that distribution.
- The output is equal to the state (that is g is the identity function).
- Some states (or state-action pairs) are more desirable than others.

Recall that stochastic is another word for *probabilistic*; we don't say "random" because that can be interpreted in two ways, both of which are incorrect. We don't pick the transition function itself at random from a distribution. The transition function doesn't pick its output *uniformly* at random.

An MDP can be used to model interaction with an outside "world," such as a single-player game.

We will focus on the case in which $\mathcal{S}$ and $\mathcal{X}$ are finite, and will call the input set $\mathcal{A}$ for *actions* (rather than $\mathcal{X}$). The idea is that an agent (a robot or a game-player) can model its environment as an MDP and try to choose actions that will drive the process into states that have high scores.

There is an interesting variation on MDPs, called a *partially observable* MDP, in which the output is also drawn from a distribution depending on the state.

Formally, an MDP is $\langle \mathcal{S}, \mathcal{A}, T, R, \gamma \rangle$ where:

- $T : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \to \mathbb{R}$ is a *transition model*, where

  $$T(s, a, s') = P(S_t = s' | S_{t-1} = s, A_{t-1} = a) \ ,$$

  specifying a conditional probability distribution;
- $R : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ is a reward function, where $R(s, a)$ specifies how desirable it is to be in state s and take action a; and
- $\gamma \in [0, 1]$ is a *discount factor*, which we'll discuss in section 2.2.

And there is an interesting, direct extension to two-player zero-sum games, such as Chess and Go.

A *policy* is a function $\pi : \mathcal{S} \to \mathcal{A}$ that specifies what action to take in each state.

The notation here uses capital letters, like S, to stand for random variables and small letters to stand for concrete values. So S_t here is a random variable that can take on elements of $\mathcal{S}$ as values.

2.1 Finite-horizon solutions

Given an MDP, our goal is typically to find a policy that is optimal in the sense that it gets as much total reward as possible, in expectation over the stochastic transitions that the domain makes. In this section, we will consider the case where there is a finite *horizon* H, indicating the total number of steps of interaction that the agent will have with the MDP.

2.1.1 Evaluating a given policy

Before we can talk about how to find a good policy, we have to specify a measure of the goodness of a policy. We will do so by defining for a given MDP policy π and horizon h, the "horizon h *value*" of a state, $V_\pi^h(s)$. We do this by induction on the horizon, which is the *number of steps left to go*.

The base case is when there are no steps remaining, in which case, no matter what state we're in, the value is 0, so

$$V_\pi^0(s) = 0 \ .$$

Then, the value of a policy in state s at horizon $h+1$ is equal to the reward it will get in state s plus the next state's expected horizon h value. So, starting with horizons 1 and 2, and then moving to the general case, we have:

$$\begin{aligned}
V_\pi^1(s) &= R(s, \pi(s)) + 0 \\
V_\pi^2(s) &= R(s, \pi(s)) + \sum_{s'} T(s, \pi(s), s') \cdot R(s', \pi(s')) \\
&\vdots \\
V_\pi^h(s) &= R(s, \pi(s)) + \sum_{s'} T(s, \pi(s), s') \cdot V_\pi^{h-1}(s')
\end{aligned}$$

The sum over s' is an *expected value*: it considers all possible next states s', and computes an average of their $(h-1)$-horizon values, weighted by the probability that the transition function from state s with the action chosen by the policy, $\pi(s)$, assigns to arriving in state s'.

Study Question: What is $\sum_{s'} T(s, a, s')$ for any particular s and a?

Then we can say that a policy π_1 is better than policy π_2 for horizon h, i.e. $\pi_1 >_h \pi_2$, if and only if for all $s \in \mathcal{S}$, $V_{\pi_1}^h(s) \geqslant V_{\pi_2}^h(s)$ and there exists at least one $s \in \mathcal{S}$ such that $V_{\pi_1}^h(s) > V_{\pi_2}^h(s)$.

2.1.2 Finding an optimal policy

How can we go about finding an optimal policy for an MDP? We could imagine enumerating all possible policies and calculating their value functions as in the previous section and picking the best one...but that's too much work!

The first observation to make is that, in a finite-horizon problem, the best action to take depends on the current state, but also on the horizon: imagine that you are in a situation where you could reach a state with reward 5 in one step or a state with reward 10 in two steps. If you have at least two steps to go, then you'd move toward the reward 10 state, but if you only have step left to go, you should go in the direction that will allow you to gain 5!

One way to find an optimal policy is to compute an *optimal action-value function*, Q. For the finite-horizon case, we define $Q^h(s, a)$ to be the expected value of

- starting in state s,

- executing action a, and
- continuing for $h-1$ more steps executing an optimal policy for the appropriate horizon on each step.

Similar to our definition of V^h for evaluating a policy, we define the Q^h function recursively according to the horizon. The only difference is that, on each step with horizon h, rather than selecting an action specified by a given policy, we select the value of a that will maximize the expected Q^h value of the next state.

$$\begin{aligned}
Q^0(s,a) &= 0 \\
Q^1(s,a) &= R(s,a) + 0 \\
Q^2(s,a) &= R(s,a) + \sum_{s'} T(s,a,s') \max_{a'} R(s',a') \\
&\vdots \\
Q^h(s,a) &= R(s,a) + \sum_{s'} T(s,a,s') \max_{a'} Q^{h-1}(s',a')
\end{aligned}$$

We can solve for the values of Q^h with a simple recursive algorithm called *finite-horizon value iteration* which just computes Q^h starting from horizon 0 and working backward to the desired horizon H. Given Q^h, an optimal finite-horizon policy π^*_h is easy to find:

$$\pi^*_h(s) = \arg\max_a Q^h(s,a) \quad .$$

There may be multiple possible optimal policies.

Dynamic programming (somewhat counter-intuitively, dynamic programming is neither really "dynamic" nor a type of "programming" as we typically understand it) is a technique for designing efficient algorithms. Most methods for solving MDPs or computing value functions rely on dynamic programming to be efficient.
The *principle of dynamic programming* is to compute and store the solutions to simple sub-problems that can be re-used later in the computation. It is a very important tool in our algorithmic toolbox.
Let's consider what would happen if we tried to compute $Q^4(s,a)$ for all (s,a) by directly using the definition:

- To compute $Q^4(s_i,a_j)$ for any one (s_i,a_j), we would need to compute $Q^3(s,a)$ for all (s,a) pairs.
- To compute $Q^3(s_i,a_j)$ for any one (s_i,a_j), we'd need to compute $Q^2(s,a)$ for all (s,a) pairs.
- To compute $Q^2(s_i,a_j)$ for any one (s_i,a_j), we'd need to compute $Q^1(s,a)$ for all (s,a) pairs.
- Luckily, those are just our $R(s,a)$ values.

So, if we have n states and m actions, this is $O((mn)^3)$ work—that seems like way too much, especially as the horizon increases! But observe that we really only have mnh values that need to be computed, $Q^h(s,a)$ for all h,s,a. If we start with $h=1$, compute and store those values, then using and reusing the $Q^{h-1}(s,a)$ values to compute the $Q^h(s,a)$ values, we can do all this computation in time $O(mnh)$, which is much better!

2.2 Infinite-horizon solutions

It is more typical to work in a regime where the actual finite horizon is not known. This is called the *infinite horizon* version of the problem, when you don't know when the game will be over! However, if we tried to simply take our definition of Q^h above and set $h = \infty$, we would be in trouble, because it could well be that the Q^∞ values for all actions would be infinite, and there would be no way to select one over the other.

There are two standard ways to deal with this problem. One is to take a kind of *average* over all time steps, but this can be a little bit tricky to think about. We'll take a different approach, which is to consider the *discounted* infinite horizon. We select a discount factor $0 < \gamma < 1$. Instead of trying to find a policy that maximizes expected finite-horizon undiscounted value,

$$\mathbb{E}\left[\sum_{t=0}^{h} R_t \mid \pi, s_0\right] ,$$

we will try to find one that maximizes the expected *infinite horizon discounted value*, which is

$$\mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t R_t \mid \pi, S_0\right] = \mathbb{E}\left[R_0 + \gamma R_1 + \gamma^2 R_2 + \ldots \mid \pi, s_0\right] .$$

Note that the t indices here are not the number of steps to go, but actually the number of steps forward from the starting state (there is no sensible notion of "steps to go" in the infinite horizon case).

There are two good intuitive motivations for discounting. One is related to economic theory and the present value of money: you'd generally rather have some money today than that same amount of money next week (because you could use it now or invest it). The other is to think of the whole process terminating, with probability $1 - \gamma$ on each step of the interaction. This value is the expected amount of reward the agent would gain under this terminating model.

2.2.1 Evaluating a policy

We will start, again, by evaluating a policy, but now in terms of the expected discounted infinite-horizon value that the agent will get in the MDP if it executes that policy. We define the infinite-horizon value of a state s under policy π as

$$V_\pi(s) = \mathbb{E}[R_0 + \gamma R_1 + \gamma^2 R_2 + \cdots \mid \pi, S_0 = s] = \mathbb{E}[R_0 + \gamma(R_1 + \gamma(R_2 + \gamma \ldots))) \mid \pi, S_0 = s] .$$

Because the expectation of a linear combination of random variables is the linear combination of the expectations, we have

$$\begin{aligned} V_\pi(s) &= \mathbb{E}[R_0 \mid \pi, S_0 = s] + \gamma \mathbb{E}[R_1 + \gamma(R_2 + \gamma \ldots))) \mid \pi, S_0 = s] \\ &= R(s, \pi(s)) + \gamma \sum_{s'} T(s, \pi(s), s') V_\pi(s') \end{aligned}$$

You could write down one of these equations for each of the $n = |\mathcal{S}|$ states. There are n unknowns $V_\pi(s)$. These are linear equations, and so it's easy to solve them using Gaussian elimination to find the value of each state under this policy.

This is *so* cool! In a discounted model, if you find that you survived this round and landed in some state s', then you have the same expected future lifetime as you did before. So the value function that is relevant in that state is exactly the same one as in state s.

2.2.2 Finding an optimal policy

The best way of behaving in an infinite-horizon discounted MDP is not time-dependent: at every step, your expected future lifetime, given that you have survived until now, is $1/(1-\gamma)$.

Study Question: Verify this fact: if, on every day you wake up, there is a probability of $1-\gamma$ that today will be your last day, then your expected lifetime is $1/(1-\gamma)$ days.

An important theorem about MDPs is: in the infinite-horizon case, there exists a stationary optimal policy π^* (there may be more than one) such that for all $s \in \mathcal{S}$ and all other policies π, we have

$$V_{\pi^*}(s) \geqslant V_{\pi}(s) \quad .$$

Stationary means that it doesn't change over time; in contrast, the optimal policy in a finite-horizon MDP is *non-stationary.*

There are many methods for finding an optimal policy for an MDP. We have already seen the finite-horizon value iteration case. Here we will study a very popular and useful method for the infinite-horizon case, *infinite-horizon value iteration*. It is also important to us, because it is the basis of many *reinforcement-learning* methods.

Define $Q^*(s,a)$ to be the expected infinite-horizon discounted value of being in state s, executing action a, and executing an optimal policy π^* thereafter. Using similar reasoning to the recursive definition of V_π, we can express this value recursively as

$$Q^*(s,a) = R(s,a) + \gamma \sum_{s'} T(s,a,s') \max_{a'} Q^*(s',a') \quad .$$

This is also a set of equations, one for each (s,a) pair. This time, though, they are not linear, and so they are not easy to solve. But there is a theorem that says they have a unique solution!

If we knew the optimal action-value function, then we could derive an optimal policy π^* as

$$\pi^*(s) = \arg\max_a Q^*(s,a) \quad .$$

Study Question: The optimal value function is unique, but the optimal policy is not. Think of a situation in which there is more than one optimal policy.

We can iteratively solve for the Q^* values with the infinite-horizon value iteration algorithm, shown below:

INFINITE-HORIZON-VALUE-ITERATION$(\mathcal{S}, \mathcal{A}, T, R, \gamma, \epsilon)$

for $s \in \mathcal{S}, a \in \mathcal{A}$:
    $Q_{\text{old}}(s,a) = 0$
while True:
    for $s \in \mathcal{S}, a \in \mathcal{A}$:
        $Q_{\text{new}}(s,a) = R(s,a) + \gamma \sum_{s'} T(s,a,s') \max_{a'} Q_{\text{old}}(s',a')$
    if $\max_{s,a} |Q_{\text{old}}(s,a) - Q_{\text{new}}(s,a)| < \epsilon$:
        return Q_{new}
    $Q_{\text{old}} = Q_{\text{new}}$

2.2.3 Theory

There are a lot of nice theoretical results about infinite-horizon value iteration. For some given (not necessarily optimal) Q function, define $\pi_Q(s) = \arg\max_a Q(s,a)$.

- After executing infinite-horizon value iteration with parameter ϵ,

$$\|V_{\pi_{Q_{\text{new}}}} - V_{\pi^*}\|_{\max} < \epsilon \quad .$$

This is new notation! Given two functions f and f', we write $\|f - f'\|_{\max}$ to mean $\max_x |f(x) - f'(x)|$. It measures the maximum absolute disagreement between the two functions at any input x.

- There is a value of ϵ such that

$$\|Q_{\text{old}} - Q_{\text{new}}\|_{\max} < \epsilon \implies \pi_{Q_{\text{new}}} = \pi^*$$

- As the algorithm executes, $\|V_{\pi_{Q_{\text{new}}}} - V_{\pi^*}\|_{\max}$ decreases monotonically on each iteration.
- The algorithm can be executed asynchronously, in parallel: as long as all (s, a) pairs are updated infinitely often in an infinite run, it still converges to optimal value.

This is very important for reinforcement learning.

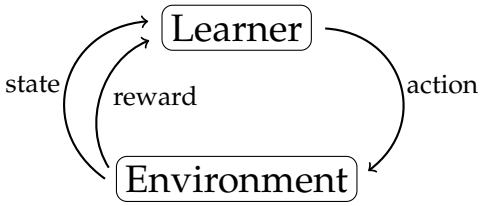
CHAPTER 11

Reinforcement learning

So far, all the learning problems we have looked at have been *supervised*: that is, for each training input $x^{(i)}$, we are told which value $y^{(i)}$ should be the output. A very different problem setting is *reinforcement learning*, in which the learning system is not directly told which outputs go with which inputs. Instead, there is an interaction of the form:

- Learner observes *input* $s^{(i)}$
- Learner generates *output* $a^{(i)}$
- Learner observes *reward* $r^{(i)}$
- Learner observes *input* $s^{(i+1)}$
- Learner generates *output* $a^{(i+1)}$
- Learner observes *reward* $r^{(i+1)}$
- ...

The learner is supposed to find a *policy*, mapping s to a, that maximizes expected reward over time.



This problem setting is equivalent to an *online* supervised learning under the following assumptions:

1. The space of possible outputs is binary (e.g. $\{+1, -1\}$) and the space of possible rewards is binary (e.g. $\{+1, -1\}$);
2. $s^{(i)}$ is independent of all previous $s^{(j)}$ and $a^{(j)}$; and
3. $r^{(i)}$ depends only on $s^{(i)}$ and $a^{(i)}$.

In this case, for any experience tuple $(s^{(i)}, a^{(i)}, r^{(i)})$, we can generate a supervised training example, which is equal to $(s^{(i)}, a^{(i)})$ if $r^{(i)} = +1$ and $(s^{(i)}, -a^{(i)})$ otherwise.

Study Question: What supervised-learning loss function would this objective correspond to?

Reinforcement learning is more interesting when these properties do not hold. When we relax assumption 1 above, we have the class of *bandit problems*, which we will discuss in section 1. If we relax assumption 2, but assume that the environment that the agent is interacting with is an MDP, so that $s^{(i)}$ depends only on $s^{(i-1)}$ and $a^{(i-1)}$ then we are in the classical *reinforcement-learning* setting, which we discuss in section 2. Weakening the assumptions further, for instance, not allowing the learner to observe the current state completely and correctly, makes the problem into a *partially observed MDP* (POMDP), which is substantially more difficult, and beyond the scope of this class.

1 Bandit problems

A basic bandit problem is given by

- A set of actions $\mathcal{A}$;
- A set of reward values $\mathcal{R}$; and
- A probabilistic reward function $R : \mathcal{A} \times \mathcal{R} \to \mathbb{R}$, i.e. R is a function that takes an action and a reward and returns the probability of getting that reward conditioned on that action being taken, $R(a, r) = p(\text{reward} = r \,|\, \text{action} = a)$. This is analogous to how the transition function T is defined. Each time the agent takes an action, a new value is drawn from this distribution.

The most typical bandit problem has $\mathcal{R} = \{0, 1\}$ and $|\mathcal{A}| = k$. This is called a k-*armed bandit problem*. There is a lot of mathematical literature on optimal strategies for k-armed bandit problems under various assumptions. The important question is usually one of *exploration versus exploitation*. Imagine that you have tried each action 10 times, and now you have estimates $\hat{R}(a_j, r)$ for the probabilities $R(a_j, r)$ for reward r given action a_j. Which arm should you pick next? You could

Why? Because in English slang, "one-armed bandit" is a name for a slot machine (an old-style gambling machine where you put a coin into a slot and then pull its arm to see if you get a payoff.) because it has one arm and takes your money! What we have here is a similar sort of machine, but with k arms.

exploit your knowledge, and choose the arm with the highest value of $\hat{R}(a_j, r)$ on all future trials; or

explore further, by trying some or all actions more times, hoping to get better estimates of the $R(a_j, r)$ values.

The theory ultimately tells us that, the longer our horizon H (or, similarly, closer to 1 our discount factor), the more time we should spend exploring, so that we don't converge prematurely on a bad choice of action.

Study Question: Why is it that "bad" luck during exploration is more dangerous than "good" luck? Imagine that there is an action that generates reward value 1 with probability 0.9, but the first three times you try it, it generates value 0. How might that cause difficulty? Why is this more dangerous than the situation when an action that generates reward value 1 with probability 0.1 actually generates reward 1 on the first three tries?

Note that what makes this a very different kind of problem from the batch supervised learning setting is that:

- The agent gets to influence what data it gets (selecting a_j gives it another sample from $R(a_j, r)$), and
- The agent is penalized for mistakes it makes while it is learning (if it is trying to maximize the expected reward $\sum_r r R(a_j, r)$ it gets while behaving).

There is a setting of supervised learning, called *active learning*, where instead of being given a training set, the learner gets to select values of x and the environment gives back a label y; the problem of picking good x values to query is interesting, but the problem of deriving a hypothesis from (x, y) pairs is the same as the supervised problem we have been studying.

In a *contextual* bandit problem, you have multiple possible states, drawn from some set $\mathcal{S}$, and a separate bandit problem associated with each one.

Bandit problems will be an essential sub-component of reinforcement learning.

2 Sequential problems

In the more typical (and difficult!) case, we can think of our learning agent interacting with an MDP, where it knows $\mathcal{S}$ and $\mathcal{A}$, but not $T(s, a, s')$ or $R(s, a)$. The learner can interact with the environment by selecting actions. So, this is somewhat like a contextual bandit problem, but more complicated, because selecting an action influences not only what the immediate reward will be, but also what state the system ends up in at the next time step and, therefore, what additional rewards might be available in the future. Note that for simplicity, in the following we will use the deterministic reward function $R(s, a)$ defined in the last chapter, rather than the probabilistic one defined above for the bandit problem.

A *reinforcement-learning (RL) algorithm* is a kind of a policy that depends on the whole history of states, actions, and rewards and selects the next action to take. There are several different ways to measure the quality of an RL algorithm, including:

- Ignoring the r_t values that it gets *while* learning, but consider how many interactions with the environment are required for it to learn a policy $\pi : \mathcal{S} \to \mathcal{A}$ that is nearly optimal.
- Maximizing the expected discounted sum of total rewards while it is learning.

Most of the focus is on the first criterion, because the second one is very difficult. The first criterion is reasonable when the learning can take place somewhere safe (imagine a robot learning, inside the robot factory, where it can't hurt itself too badly) or in a simulated environment.

Approaches to reinforcement-learning differ significantly according to what kind of hypothesis or model they learn. In the following sections, we will consider several different approaches.

2.1 Model-based RL

The conceptually simplest approach to RL is to model R and T from the data we have gotten so far, and then use those models, together with an algorithm for solving MDPs (such as value iteration) to find a policy that is near-optimal given the current models.

Assume that we have had some set of interactions with the environment, which can be characterized as a set of tuples of the form $(s^{(t)}, a^{(t)}, r^{(t)}, s^{(t+1)})$.

Because the transition function $T(s, a, s')$ specifies probabilities, multiple observations of (s, a, s') may be needed to model the function. One approach to this task of building a model $\hat{T}(s, a, s')$ for the true $T(s, a, s')$ is to estimate it using a simple counting strategy,

$$\hat{T}(s, a, s') = \frac{\#(s, a, s') + 1}{\#(s, a) + |\mathcal{S}|}.$$

Here, $\#(s, a, s')$ represents the number of times in our data set we have the situation where $s_t = s, a_t = a, s_{t+1} = s'$ and $\#(s, a)$ represents the number of times in our data set we have the situation where $s_t = s, a_t = a$.

Study Question: Prove to yourself that $\#(s, a) = \sum_{s'} \#(s, a, s')$.

Adding 1 and $|\mathcal{S}|$ to the numerator and denominator, respectively, are a form of smoothing called the *Laplace correction*. It ensures that we never estimate that a probability is 0,

and keeps us from dividing by 0. As the amount of data we gather increases, the influence of this correction fades away.

In contrast, the reward function $R(s, a)$ (as we have specified it in this text) is a *deterministic* function, such that knowing the reward r for a given (s, a) is sufficient to fully determine the function at that point. In other words, our model $\hat{R}$ can simply be a record of observed rewards, such that $\hat{R}(s, a) = r = R(s, a)$.

A more general case is when the reward function is *non-deterministic*, such that the reward $R(s, a)$ may vary with each query. In this case, an estimation strategy similar to that employed for the model $\hat{T}$ could be used for building the model $\hat{R}$, e.g.:

$$\hat{R}(s, a) = \frac{\sum r \mid s, a}{\#(s, a)}$$

where

$$\sum r \mid s, a = \sum_{\{t | s_t = s, a_t = a\}} r^{(t)} \ .$$

Such an estimate would just be the average of the observed rewards for each s, a pair. However, this general case is outside the scope of what we will cover here.

Given empirical models $\hat{T}$ and $\hat{R}$ for the transition and reward functions, we can now solve the MDP $(S, A, \hat{T}, \hat{R})$ to find an optimal policy using value iteration, or use a finite-depth expecti-max search to find an action to take for a particular state.

This technique is effective for problems with small state and action spaces, where it is not too hard to get enough experience to model T and R well; but it is difficult to generalize this method to handle continuous (or very large discrete) state spaces, and is a topic of current research.

2.2 Policy search

A very different strategy is to search directly for a good policy, without first (or ever!) estimating the transition and reward models. The strategy here is to define a functional form $f(s; \theta) = a$ for the policy, where θ represents the parameters we learn from experience. We choose f to be differentiable, and often let $f(s; \theta) = P(a)$, a probability distribution over our possible actions.

Now, we can train the policy parameters using gradient descent:

- When θ has relatively low dimension, we can compute a numeric estimate of the gradient by running the policy multiple times for $\theta \pm \epsilon$, and computing the resulting rewards.
- When θ has higher dimensions (e.g., it is a complicated neural network), there are more clever algorithms, e.g., one called REINFORCE, but they can often be difficult to get to work reliably.

Policy search is a good choice when the policy has a simple known form, but the model would be much more complicated to estimate.

2.3 Value function learning

The most popular class of algorithms learns neither explicit transition and reward models nor a direct policy, but instead concentrates on learning a value function. It is a topic of current research to describe exactly under what circumstances value-function-based approaches are best, and there are a growing number of methods that combine value functions, transition and reward models and policies into a complex learning algorithm in an attempt to combine the strengths of each approach.

We will study two variations on value-function learning, both of which estimate the Q function.

2.3.1 Q-learning

This is the most typical way of performing reinforcement learning. Recall the value-iteration update:

$$Q(s,a) = R(s,a) + \gamma \sum_{s'} T(s,a,s') \max_{a'} Q(s',a')$$

The thing that most students seem to get confused about is when we do value iteration and when we do Q learning. Value iteration assumes you know T and R and just need to *compute* Q. In Q learning, we don't know or even directly estimate T and R: we estimate Q directly from experience!

We will adapt this update to the RL scenario, where we do not know the transition function T or reward function R.

Q-LEARNING($\mathcal{S}, \mathcal{A}, s_0, \gamma, \alpha$)

```
1  for s ∈ S, a ∈ A :
2      Q[s, a] = 0
3  s = s_0 // Or draw an s randomly from S
4  while True:
5      a = select_action(s, Q)
6      r, s' = execute(a)
7      Q[s, a] = (1 − α)Q[s, a] + α(r + γ max_a' Q[s', a'])
8      s = s'
```

Here, α represents the "learning rate," which needs to decay for convergence purposes, but in practice is often set to a constant.

Note that the update can be rewritten as

$$Q[s,a] = Q[s,a] - \alpha \left(Q[s,a] - (r + \gamma \max_{a'} Q[s',a']) \right),$$

which looks something like a gradient update! This is often called *temporal difference* learning method, because we make an update based on the difference between the current estimated value of taking action a in state s, which is $Q[s,a]$, and the "one-step" sampled value of taking a in s, which is $r + \gamma \max_{a'} Q[s',a']$.

It is actually not a gradient update, but later, when we consider function approximation, we will treat it as if it were.

You can see this method as a combination of two different iterative processes that we have already seen: the combination of an old estimate with a new sample using a running average with a learning rate α, and the dynamic-programming update of a Q value from value iteration.

Our algorithm above includes a procedure called *select_action*, which, given the current state s, has to decide which action to take. If the Q value is estimated very accurately and the agent is behaving in the world, then generally we would want to choose the apparently optimal action $\arg\max_{a \in \mathcal{A}} Q(s,a)$. But, during learning, the Q value estimates won't be very good and exploration is important. However, exploring completely at random is also usually not the best strategy while learning, because it is good to focus your attention on the parts of the state space that are likely to be visited when executing a good policy (not a stupid one).

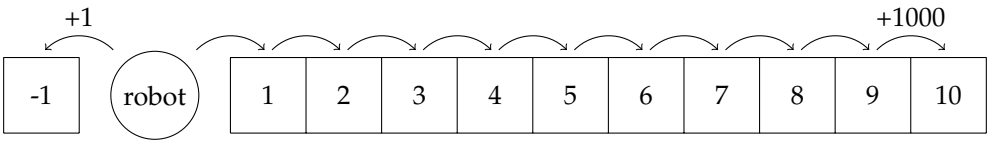
A typical action-selection strategy is the ϵ-greedy strategy:

- with probability $1 - \epsilon$, choose $\arg\max_{a \in \mathcal{A}} Q(s,a)$
- with probability ϵ, choose the action $a \in \mathcal{A}$ uniformly at random

Q-learning has the surprising property that it is *guaranteed* to converge to the actual optimal Q function under fairly weak conditions! Any exploration strategy is okay as

long as it tries every action infinitely often on an infinite run (so that it doesn't converge prematurely to a bad action choice).

Q-learning can be very sample-inefficient: imagine a robot that has a choice between moving to the left and getting a reward of 1, then returning to its initial state, or moving to the right and walking down a 10-step hallway in order to get a reward of 1000, then returning to its initial state.



The first time the robot moves to the right and goes down the hallway, it will update the Q value for the last state on the hallway to have a high value, but it won't yet understand that moving to the right was a good choice. The next time it moves down the hallway it updates the value of the state before the last one, and so on. After 10 trips down the hallway, it now can see that it is better to move to the right than to the left.

More concretely, consider the vector of Q values $Q(0:10, \text{right})$, representing the Q values for moving right at each of the positions $0, \ldots, 9$. Then, for $\alpha = 1$ and $\gamma = 0.9$,

$$Q(i, \text{right}) = R(i, \text{right}) + 0.9 \cdot \max_a Q(i+1, a)$$

Starting with Q values of 0,

$$Q^{(0)}(0:10, \text{right}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Since the only nonzero reward from moving right is $R(9, \text{right}) = 1000$, after our robot makes it down the hallway once, our new Q vector is

$$Q^{(1)}(0:10, \text{right}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1000 & 0 \end{bmatrix}$$

After making its way down the hallway again, $Q(8, \text{right}) = 0 + 0.9 \cdot Q(9, \text{right}) = 900$ updates:

$$Q^{(2)}(0:10, \text{right}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 900 & 1000 & 0 \end{bmatrix}$$

Similarly,

$$\begin{aligned} Q^{(3)}(0:10, \text{right}) &= \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 810 & 900 & 1000 & 0 \end{bmatrix} \\ Q^{(4)}(0:10, \text{right}) &= \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 729 & 810 & 900 & 1000 & 0 \end{bmatrix} \\ &\vdots \\ Q^{(10)}(0:10, \text{right}) &= \begin{bmatrix} 387.4 & 420.5 & 478.3 & 531.4 & 590.5 & 656.1 & 729 & 810 & 900 & 1000 & 0 \end{bmatrix}, \end{aligned}$$

and the robot finally sees the value of moving right from position 0.

We are violating our usual notational conventions here, and writing $Q^{(i)}$ to mean the Q value function that results after the robot runs all the way to the end of the hallway, when executing the policy that always moves to the right.

We can see how this interacts with the exploration/exploitation dilemma: from the perspective of s_0, it will seem, for a long time, that getting the immediate reward of 1 is a better idea, and it would be easy to converge on that as a strategy without exploring the long hallway sufficiently.

Study Question: Determine the Q value functions that will result from updates due to the robot always executing the "move left" policy.

2.3.2 Function approximation

In our Q-learning algorithm above, we essentially keep track of each Q value in a table, indexed by s and a. What do we do if $\mathcal{S}$ and/or $\mathcal{A}$ are large (or continuous)?

We can use a function approximator like a neural network to store Q values. For example, we could design a neural network that takes in inputs s and a, and outputs $Q(s, a)$. We can treat this as a regression problem, optimizing the squared Bellman error, with loss:

$$\left(Q(s, a) - (r + \gamma \max_{a'} Q(s', a'))\right)^2 ,$$

where $Q(s, a)$ is now the output of the neural network.

There are actually several different architectural choices for using a neural network to approximate Q values:

- One network for each action a_j, that takes s as input and produces $Q(s, a_j)$ as output;
- One single network that takes s as input and produces a vector $Q(s, \cdot)$, consisting of the Q values for each action; or
- One single network that takes s, a concatenated into a vector (if a is discrete, we would probably use a one-hot encoding, unless it had some useful internal structure) and produces $Q(s, a)$ as output.

The first two choices are only suitable for discrete (and not too big) action sets. The last choice can be applied for continuous actions, but then it is difficult to find $\arg\max_A Q(s, a)$.

For continuous action spaces, it is increasingly popular to use a class of methods called *actor-critic* methods, which combine policy and value-function learning. We won't get into them in detail here, though.

There are not many theoretical guarantees about Q-learning with function approximation and, indeed, it can sometimes be fairly unstable (learning to perform well for a while, and then getting suddenly worse, for example). But it has also had some significant successes.

One form of instability that we do know how to guard against is *catastrophic forgetting*. In standard supervised learning, we expect that the training x values were drawn independently from some distribution. But when a learning agent, such as a robot, is moving through an environment, the sequence of states it encounters will be temporally correlated. This can mean that while it is in the dark, the neural-network weight-updates will make the Q function "forget" the value function for when it's light.

And, in fact, we routinely shuffle their order in the data file, anyway.

For example, it might spend 12 hours in a dark environment and then 12 in a light one.

One way to handle this is to use *experience replay*, where we save our (s, a, r, s') experiences in a *replay buffer*. Whenever we take a step in the world, we add the (s, a, r, s') to the replay buffer and use it to do a Q-learning update. Then we also randomly select some number of tuples from the replay buffer, and do Q-learning updates based on them, as well. In general it may help to keep a *sliding window* of just the 1000 most recent experiences in the replay buffer. (A larger buffer will be necessary for situations when the optimal policy might visit a large part of the state space, but we like to keep the buffer size small for memory reasons and also so that we don't focus on parts of the state space that are irrelevant for the optimal policy.) The idea is that it will help you propagate reward values through your state space more efficiently if you do these updates. You can see it as doing something like value iteration, but using samples of experience rather than a known model.

2.3.3 Fitted Q-learning

An alternative strategy for learning the Q function that is somewhat more robust than the standard Q-learning algorithm is a method called *fitted Q*.

FITTED-Q-LEARNING($\mathcal{A}, s_0, \gamma, \alpha, \epsilon, m$)

```
1  s = s_0 // Or draw an s randomly from S
2  D = { }
3  initialize neural-network representation of Q
4  while True:
5      D_new = experience from executing ε-greedy policy based on Q for m steps
6      D = D ∪ D_new represented as (s, a, r, s') tuples
7      D_sup = {(x^(i), y^(i))} where x^(i) = (s, a) and y^(i) = r + γ max_{a'∈A} Q(s', a')
8        for each tuple (s, a, r, s')^(i) ∈ D
9      re-initialize neural-network representation of Q
10     Q = supervised_NN_regression(D_sup)
```

Here, we alternate between using the policy induced by the current Q function to gather a batch of data $\mathcal{D}_{\text{new}}$, adding it to our overall data set $\mathcal{D}$, and then using supervised neural-network training to learn a representation of the Q value function on the whole data set. This method does not mix the dynamic-programming phase (computing new Q values based on old ones) with the function approximation phase (training the neural network) and avoids catastrophic forgetting. The regression training in line 9 typically uses squared error as a loss function and would be trained until the fit is good (possibly measured on held-out data).

CHAPTER 12

Recurrent Neural Networks

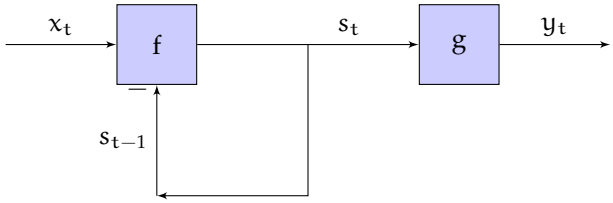
In chapter 8 we studied neural networks and how we can train the weights of a network, based on data, so that it will adapt into a function that approximates the relationship between the (x, y) pairs in a supervised-learning training set. In section 1 of chapter 10, we studied state-machine models and defined *recurrent neural networks* (RNNs) as a particular type of state machine, with a multidimensional vector of real values as the state. In this chapter, we'll see how to use gradient-descent methods to train the weights of an RNN so that it performs a *transduction* that matches as closely as possible a training set of input-output *sequences*.

1 RNN model

Recall that the basic operation of the state machine is to start with some state s_0, then iteratively compute for $t \geqslant 1$::

$$s_t = f(s_{t-1}, x_t)$$
$$y_t = g(s_t)$$

as illustrated in the diagram below (remembering that there needs to be a delay on the feedback loop):



So, given a sequence of inputs $x_1, x_2, \ldots$ the machine generates a sequence of outputs

$$\underbrace{g(f(s_0, x_1))}_{y_1}, \underbrace{g(f(f(s_0, x_1), x_2))}_{y_2}, \ldots \quad .$$

A *recurrent neural network* is a state machine with neural networks constituting functions f and g:

$$f(s, x) = f_1(W^{sx}x + W^{ss}s + W_0^{ss})$$
$$g(s) = f_2(W^o s + W_0^o) \ .$$

The inputs, states, and outputs are all vector-valued:

$$x_t : \ell \times 1$$
$$s_t : m \times 1$$
$$y_t : n \times 1 \ .$$

We are very sorry! This course material has evolved from different sources, which used $W^T x$ in the forward pass for regular feed-forward NNs and Wx for the forward pass in RNNs. This inconsistency doesn't make any technical difference, but is a potential source of confusion.

The weights in the network, then, are

$$W^{sx} : m \times \ell$$
$$W^{ss} : m \times m$$
$$W_0^{ss} : m \times 1$$
$$W^o : n \times m$$
$$W_0^o : n \times 1$$

with activation functions f_1 and f_2. Finally, the operation of the RNN is described by

$$s_t = f_1\left(W^{sx}x_t + W^{ss}s_{t-1} + W_0^{ss}\right)$$
$$y_t = f_2\left(W^o s_t + W_0^o\right) \ .$$

Study Question: Check dimensions here to be sure it all works out. Remember that we apply f_1 and f_2 elementwise.

2 Sequence-to-sequence RNN

Now, how can we train an RNN to model a transduction on sequences? This problem is sometimes called *sequence-to-sequence* mapping. You can think of it as a kind of regression problem: given an input sequence, learn to generate the corresponding output sequence.

A training set has the form $\left[\left(x^{(1)}, y^{(1)}\right), \ldots, \left(x^{(q)}, y^{(q)}\right)\right]$, where

- $x^{(i)}$ and $y^{(i)}$ are length $n^{(i)}$ sequences;
- sequences in the *same pair* are the same length; and sequences in different pairs may have different lengths.

One way to think of training a sequence **classifier** is to reduce it to a transduction problem, where $y_t = 1$ if the sequence $x_1, \ldots, x_t$ is a *positive* example of the class of sequences and -1 otherwise.

Next, we need a loss function. We start by defining a loss function on sequences. There are many possible choices, but usually it makes sense just to sum up a per-element loss function on each of the output values, where p is the predicted sequence and y is the actual one:

$$L_{seq}\left(p^{(i)}, y^{(i)}\right) = \sum_{t=1}^{n^{(i)}} L_{elt}\left(p_t^{(i)}, y_t^{(i)}\right) \ .$$

The per-element loss function L_{elt} will depend on the type of y_t and what information it is encoding, in the same way as for a supervised network.. Then, letting $\theta = (W^{sx}, W^{ss}, W^o, W_0^{ss}, W_0^o)$

So it could be NLL, squared loss, etc.

our overall objective is to minimize

$$J(\theta) = \sum_{i=1}^{q} L_{seq}\left(\text{RNN}(x^{(i)};\theta), y^{(i)}\right) \quad ,$$

where $\text{RNN}(x;\theta)$ is the output sequence generated, given input sequence x.

It is typical to choose f_1 to be *tanh* but any non-linear activation function is usable. We choose f_2 to align with the types of our outputs and the loss function, just as we would do in regular supervised learning.

Remember that it looks like a sigmoid but ranges from -1 to +1.

3 Back-propagation through time

Now the fun begins! We can find θ to minimize J using gradient descent. We will work through the simplest method, *back-propagation through time* (BPTT), in detail. This is generally not the best method to use, but it's relatively easy to understand. In section 5 we will sketch alternative methods that are in much more common use.

Calculus reminder: total derivative Most of us are not very careful about the difference between the *partial derivative* and the *total derivative*. We are going to use a nice example from the Wikipedia article on partial derivatives to illustrate the difference. The volume of a circular cone depends on its height and radius:

$$V(r,h) = \frac{\pi r^2 h}{3} \quad .$$

The partial derivatives of volume with respect to height and radius are

$$\frac{\partial V}{\partial r} = \frac{2\pi r h}{3} \quad \text{and} \quad \frac{\partial V}{\partial h} = \frac{\pi r^2}{3} \quad .$$

They measure the change in V assuming everything is held constant except the single variable we are changing. Now assume that we want to preserve the cone's proportions in the sense that the ratio of radius to height stay constant, then we can't really change one without changing the other. In this case, we really have to think about the *total derivative*, which sums the "paths" along which r might influence V:

$$\begin{aligned}
\frac{dV}{dr} &= \frac{\partial V}{\partial r} + \frac{\partial V}{\partial h}\frac{dh}{dr} \\
&= \frac{2\pi r h}{3} + \frac{\pi r^2}{3}\frac{dh}{dr} \\
\frac{dV}{dh} &= \frac{\partial V}{\partial h} + \frac{\partial V}{\partial r}\frac{dr}{dh} \\
&= \frac{\pi r^2}{3} + \frac{2\pi r h}{3}\frac{dr}{dh}
\end{aligned}$$

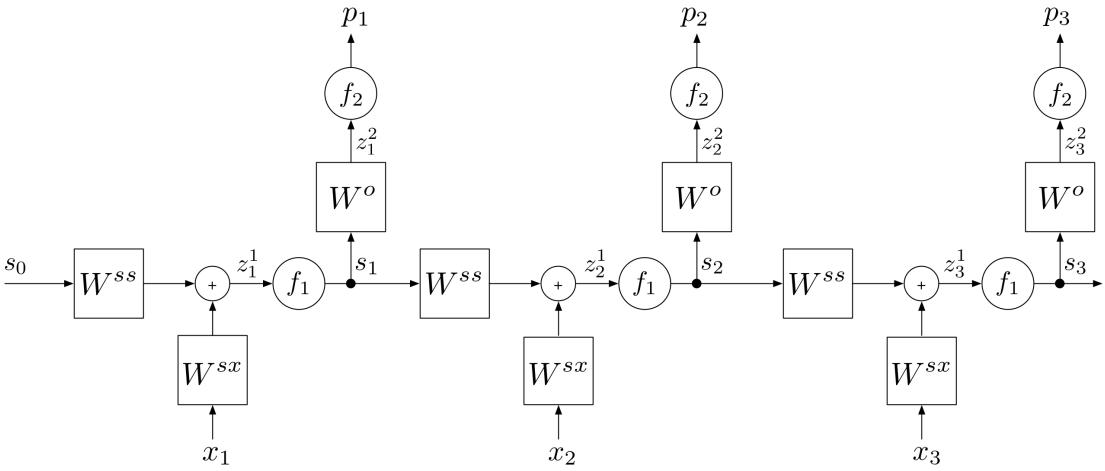
Just to be completely concrete, let's think of a right circular cone with a fixed angle $\alpha = \tan r/h$, so that if we change r or h then α remains constant. So we have $r = h\tan^{-1}\alpha$; let constant $c = \tan^{-1}\alpha$, so now $r = ch$. Thus, we finally have

$$\begin{aligned}
\frac{dV}{dr} &= \frac{2\pi r h}{3} + \frac{\pi r^2}{3}\frac{1}{c} \\
\frac{dV}{dh} &= \frac{\pi r^2}{3} + \frac{2\pi r h}{3}c \quad .
\end{aligned}$$

The BPTT process goes like this:

(1) Sample a training pair of sequences (x, y); let their length be n.

(2) "Unroll" the RNN to be length n (picture for $n = 3$ below), and initialize s_0:



Now, we can see our problem as one of performing what is almost an ordinary back-propagation training procedure in a feed-forward neural network, but with the difference that the weight matrices are shared among the layers. In many ways, this is similar to what ends up happening in a convolutional network, except in the convnet, the weights are re-used spatially, and here, they are re-used temporally.

(3) Do the *forward pass*, to compute the predicted output sequence p:

$$\begin{aligned} z_t^1 &= W^{sx} x_t + W^{ss} s_{t-1} + W_0^{ss} \\ s_t &= f_1(z_t^1) \\ z_t^2 &= W^o s_t + W_0^o \\ p_t &= f_2(z_t^2) \end{aligned}$$

(4) Do *backward pass* to compute the gradients. For both W^{ss} and W^{sx} we need to find

$$\frac{dL_{seq}(p, y)}{dW} = \sum_{u=1}^{n} \frac{dL_{elt}(p_u, y_u)}{dW} \tag{12.1}$$

Letting $L_u = L_{elt}(p_u, y_u)$ and using the *total derivative*, which is a sum over all the ways in which W affects L_u, we have

$$= \sum_{u=1}^{n} \sum_{t=1}^{n} \frac{\partial s_t}{\partial W} \cdot \frac{\partial L_u}{\partial s_t} \tag{12.2}$$

Re-organizing, we have

$$= \sum_{t=1}^{n} \frac{\partial s_t}{\partial W} \cdot \sum_{u=1}^{n} \frac{\partial L_u}{\partial s_t} \tag{12.3}$$

Because s_t only affects $L_t, L_{t+1}, \ldots, L_n$,

$$= \sum_{t=1}^{n} \frac{\partial s_t}{\partial W} \cdot \sum_{u=t}^{n} \frac{\partial L_u}{\partial s_t}$$

$$= \sum_{t=1}^{n} \frac{\partial s_t}{\partial W} \cdot \left(\frac{\partial L_t}{\partial s_t} + \underbrace{\sum_{u=t+1}^{n} \frac{\partial L_u}{\partial s_t}}_{\delta^{s_t}} \right) \tag{12.4}$$

where δ^{s_t} is the dependence of the future loss (incurred after step t) on the state S_t. We can compute this backwards, with t going from n down to 1. The trickiest part is figuring out how early states contribute to later losses. We define the *future loss* after step t to be

That is, δ^{s_t} is how much we can blame state s_t for all the future element losses.

$$F_t = \sum_{u=t+1}^{n} L_{elt}(p_u, y_u) \ ,$$

so

$$\delta^{s_t} = \frac{\partial F_t}{\partial s_t} \ .$$

At the last stage, $F_n = 0$ so $\delta^{s_n} = 0$.

Now, working backwards,

$$\begin{aligned}
\delta^{s_{t-1}} &= \frac{\partial}{\partial s_{t-1}} \sum_{u=t}^{n} L_{elt}(p_u, y_u) \\
&= \frac{\partial s_t}{\partial s_{t-1}} \cdot \frac{\partial}{\partial s_t} \sum_{u=t}^{n} L_{elt}(p_u, y_u) \\
&= \frac{\partial s_t}{\partial s_{t-1}} \cdot \frac{\partial}{\partial s_t} \left[L_{elt}(p_t, y_t) + \sum_{u=t+1}^{n} L_{elt}(p_u, y_u) \right] \\
&= \frac{\partial s_t}{\partial s_{t-1}} \cdot \left[\frac{\partial L_{elt}(p_t, y_t)}{\partial s_t} + \delta^{s_t} \right]
\end{aligned}$$

Now, we can use the chain rule again to find the dependence of the element loss at time t on the state at that same time,

$$\underbrace{\frac{\partial L_{elt}(p_t, y_t)}{\partial s_t}}_{(m \times 1)} = \underbrace{\frac{\partial z_t^2}{\partial s_t}}_{(m \times \nu)} \cdot \underbrace{\frac{\partial L_{elt}(p_t, y_t)}{\partial z_t^2}}_{(\nu \times 1)} \ ,$$

and the dependence of the state at time t on the state at the previous time,

$$\underbrace{\frac{\partial s_t}{\partial s_{t-1}}}_{(m \times m)} = \underbrace{\frac{\partial z_t^1}{\partial s_{t-1}}}_{(m \times m)} \cdot \underbrace{\frac{\partial s_t}{\partial z_t^1}}_{(m \times m)} = W^{ss\,T} \cdot \frac{\partial s_t}{\partial z_t^1}$$

Note that $\partial s_t / \partial z_t^1$ is formally an $m \times m$ diagonal matrix, with the values along the diagonal being $f_1'(z_{t,i}^1)$, $1 \leqslant i \leqslant m$. But since this is a diagonal matrix, one could represent it as an $m \times 1$ vector $f_1'(z_t^1)$. In that case the product of the matrix $W^{ss\,T}$ by the vector $f_1'(z_t^1)$, denoted $W^{ss\,T} * f_1'(z_t^1)$, should be interpreted as follows: take the first column of the matrix $W^{ss\,T}$ and multiply each of its elements by the first element of the vector $\partial s_t / \partial z_t^1$, then take the second column of the matrix $W^{ss\,T}$ and multiply each of its elements by the second element of the vector $\partial s_t / \partial z_t^1$, and so on and so for ...

Putting this all together, we end up with

$$\delta^{s_{t-1}} = \underbrace{W^{ss\,T} \cdot \frac{\partial s_t}{\partial z_t^1}}_{\frac{\partial s_t}{\partial s_{t-1}}} \cdot \underbrace{\left(W^{o\,T} \frac{\partial L_t}{\partial z_t^2} + \delta^{s_t} \right)}_{\frac{\partial F_{t-1}}{\partial s_t}}$$

We're almost there! Now, we can describe the actual weight updates. Using equation 12.4 and recalling the definition of $\delta^{s_t} = \partial F_t / \partial s_t$, as we iterate backwards, we can accumulate the terms in equation 12.4 to get the gradient for the whole loss.

$$\frac{dL_{seq}}{dW^{ss}} = \sum_{t=1}^{n} \frac{dL_{elt}(p_t, y_t)}{dW^{ss}} = \sum_{t=1}^{n} \frac{\partial z_t^1}{\partial W^{ss}} \cdot \frac{\partial s_t}{\partial z_t^1} \cdot \frac{\partial F_{t-1}}{\partial s_t}$$

$$\frac{dL_{seq}}{dW^{sx}} = \sum_{t=1}^{n} \frac{dL_{elt}(p_t, y_t)}{dW^{sx}} = \sum_{t=1}^{n} \frac{\partial z_t^1}{\partial W^{sx}} \cdot \frac{\partial s_t}{\partial z_t^1} \cdot \frac{\partial F_{t-1}}{\partial s_t}$$

We can handle W^o separately; it's easier because it does not affect future losses in the way that the other weight matrices do:

$$\frac{dL_{seq}}{dW^o} = \sum_{t=1}^{n} \frac{dL_t}{dW^o} = \sum_{t=1}^{n} \frac{\partial L_t}{\partial z_t^2} \cdot \frac{\partial z_t^2}{\partial W^o}$$

Assuming we have $\frac{\partial L_t}{\partial z_t^2} = (p_t - y_t)$, (which ends up being true for squared loss, softmax-NLL, etc.), then

$$\underbrace{\frac{dL_{seq}}{dW^o}}_{v \times m} = \sum_{t=1}^{n} \underbrace{(p_t - y_t)}_{v \times 1} \cdot \underbrace{s_t^T}_{1 \times m}$$

Whew!

Study Question: Derive the updates for the offsets W_0^{ss} and W_0^o.

4 Training a language model

A *language model* is just trained on a set of input sequences, $(c_1^{(i)}, c_2^{(i)}, \ldots, c_{n^i}^{(i)})$, and is used to predict the next character, given a sequence of previous tokens:

A "token" is generally a character or a word.

$$c_t = \text{RNN}(c_1, c_2, \ldots, c_{t-1})$$

We can convert this to a sequence-to-sequence training problem by constructing a data set of (x, y) sequence pairs, where we make up new special tokens, start and end, to signal the beginning and end of the sequence:

$$x = (\langle \text{start} \rangle, c_1, c_2, ;c_n)$$
$$y = (c_1, c_2, \ldots, \langle \text{end} \rangle)$$

5 Vanishing gradients and gating mechanisms

Let's take a careful look at the backward propagation of the gradient along the sequence:

$$\delta^{s_{t-1}} = \frac{\partial s_t}{\partial s_{t-1}} \cdot \left[\frac{\partial L_{elt}(p_t, y_t)}{\partial s_t} + \delta^{s_t} \right] \quad .$$

Consider a case where only the output at the end of the sequence is incorrect, but it depends critically, via the weights, on the input at time 1. In this case, we will multiply the loss at step n by

$$\frac{\partial s_2}{\partial s_1} \cdot \frac{\partial s_3}{\partial s_2} \cdots \frac{\partial s_n}{\partial s_{n-1}} \quad .$$

In general, this quantity will either grow or shrink exponentially with the length of the sequence, and make it very difficult to train.

Study Question: The last time we talked about exploding and vanishing gradients, it was to justify per-weight adaptive step sizes. Why is that not a solution to the problem this time?

An important insight that really made recurrent networks work well on long sequences is the idea of *gating*.

5.1 Simple gated recurrent networks

A computer only ever updates some parts of its memory on each computation cycle. We can take this idea and use it to make our networks more able to retain state values over time and to make the gradients better-behaved. We will add a new component to our network, called a *gating network*. Let g_t be a $m \times 1$ vector of values and let W^{gx} and W^{gs} be $m \times l$ and $m \times m$ weight matrices, respectively. We will compute g_t as

$$g_t = \text{sigmoid}(W^{gx} x_t + W^{gs} s_{t-1})$$

It can have an offset, too, but we are omitting it for simplicity.

and then change the computation of s_t to be

$$s_t = (1 - g_t) * s_{t-1} + g_t * f_1(W^{sx} x_t + W^{ss} s_{t-1} + W_0^{ss}) \quad ,$$

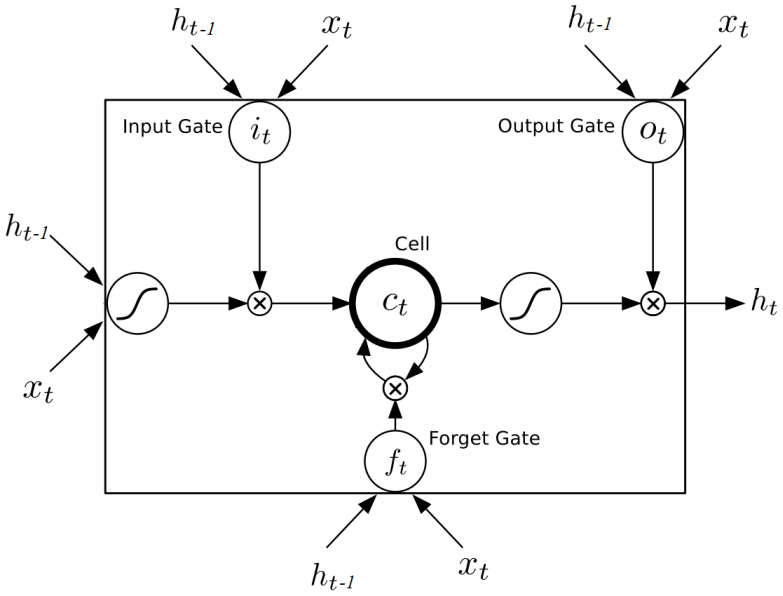
where $*$ is component-wise multiplication. We can see, here, that the output of the gating network is deciding, for each dimension of the state, how much it should be updated now. This mechanism makes it much easier for the network to learn to, for example, "store" some information in some dimension of the state, and then not change it during future state updates, or change it only under certain conditions on the input or other aspects of the state.

Study Question: Why is it important that the activation function for g be a sigmoid?

5.2 Long short-term memory

The idea of gating networks can be applied to make a state-machine that is even more like a computer memory, resulting in a type of network called an LSTM for "long short-term memory." We won't go into the details here, but the basic idea is that there is a memory cell (really, our state vector) and three (!) gating networks. The *input* gate selects (using a "soft" selection as in the gated network above) which dimensions of the state will be updated with new values; the *forget* gate decides which dimensions of the state will have its old values moved toward 0, and the *output* gate decides which dimensions of the state will be used to compute the output value. These networks have been used in applications like language translation with really amazing results. A diagram of the architecture is shown below:

Yet another awesome name for a neural network!



CHAPTER 13

Non-parametric methods

1 Intro

We will continue to broaden the class of models that we can fit to our data. Neural networks have adaptable complexity, in the sense that we can try different structural models and use cross validation to find one that works well on our data.

We now turn to models that automatically adapt their complexity to the training data. The name *non-parametric methods* is misleading: it is really a class of methods that does not have a fixed parameterization in advance. Some non-parametric models, such as decision trees, which we might call *semi-parametric methods*, can be seen as dynamically constructing something that ends up looking like a more traditional parametric model, but where the actual training data affects exactly what the form of the model will be. Other non-parametric methods, such as nearest-neighbor, rely directly on the data to make predictions and do not compute a model that summarizes the data.

The semi-parametric methods tend to have the form of a composition of simple models. We'll look at:

- *Tree models*: partition the input space and use different simple predictions on different regions of the space; this increases the hypothesis space.
- *Additive models*: train several different classifiers on the whole space and average the answers; this decreases the estimation error.

Boosting is a way to construct an additive model that decreases both estimation and structural error, but we won't address it in this class.

Why are we studying these methods, in the heyday of neural networks?

- They are fast to implement and have few or no hyper-parameters to tune.
- They often work as well or better than more complicated methods.
- Both can be easier to explain to a human user: decision-trees are fairly directly human-interpretable and nearest neighbor methods can justify their decision to some extent by showing a few training examples that the prediction was based on.

2 Trees

The idea here is that we would like to find a partition of the input space and then fit very simple models to predict the output in each piece. The partition is described using a (typically binary) "decision tree," which recursively splits the space.

These methods differ by:

- The class of possible ways to split the space at each node; these are generally linear splits, either aligned with the axes of the space, or sometimes more general classifiers.
- The class of predictors within the partitions; these are often simply constants, but may be more general classification or regression models.
- The way in which we control the complexity of the hypothesis: it would be within the capacity of these methods to have a separate partition for each individual training example.
- The algorithm for making the partitions and fitting the models.

The primary advantage of tree models is that they are easily interpretable by humans. This is important in application domains, such as medicine, where there are human experts who often ultimately make critical decisions and who need to feel confident in their understanding of recommendations made by an algorithm.

These methods are most appropriate for domains where the input space is not very high-dimensional and where the individual input features have some substantially useful information individually or in small groups. They would not be good for image input, but might be good in cases with, for example, a set of meaningful measurements of the condition of a patient in the hospital.

We'll concentrate on the CART/ID3 family of algorithms, which were invented independently in the statistics and the artificial intelligence communities. They work by greedily constructing a partition, where the splits are *axis aligned* and by fitting a *constant* model in the leaves. The interesting questions are how to select the splits and how to control complexity. The regression and classification versions are very similar.

2.1 Regression

The predictor is made up of

- a partition function, π, mapping elements of the input space into exactly one of M regions, $R_1, \ldots, R_M$, and
- a collection of M output values, O_m, one for each region.

If we already knew a division of the space into regions, we would set O_m, the constant output for region R_m, to be the average of the training output values in that region; that is:

$$O_m = \text{average}_{\{i|x^{(i)} \in R_m\}} y^{(i)} \quad .$$

Define the error in a region as

$$E_m = \sum_{\{i|x^{(i)} \in R_m\}} (y^{(i)} - O_m)^2 \quad .$$

Ideally, we would select the partition to minimize

$$\lambda M + \sum_{m=1}^{M} E_m \quad ,$$

for some regularization constant λ. It is enough to search over all partitions of the training data (not all partitions of the input space!) to optimize this, but the problem is NP-complete.

Study Question: Be sure you understand why it's enough to consider all partitions of the training data, if this is your objective.

2.1.1 Building a tree

So, we'll be greedy. We establish a criterion, given a set of data, for finding the best single split of that data, and then apply it recursively to partition the space. We will select the partition of the data that *minimizes the sum of the mean squared errors of each partition.*

Given a data set D, let

- $R^+_{j,s}(D) = \{x \in D \mid x_j \geqslant s\}$ be the set of examples in data set D whose feature value in dimension j is greater than or equal to split point s;
- $R^-_{j,s}(D) = \{x \in D \mid x_j < s\}$ be the set of examples in D whose feature value in dimension j is less than s;
- $\hat{y}^+_{j,s} = \text{average}_{\{i|x^{(i)} \in R^+_{j,s}(D)\}} y^{(i)}$ be the average y value of the data points in set $R^+_{j,s}(D)$; and
- $\hat{y}^-_{j,s} = \text{average}_{\{i|x^{(i)} \in R^-_{j,s}(D)\}} y^{(i)}$ be the average y value of the data points in set $R^-_{j,s}(D)$.

Now, here is the pseudocode.

BuildTree(D, k):

- If $|D| \leqslant k$: return Leaf(D)
- Find the dimension j and split point s that minimizes: $E_{R^-_{j,s}(D)} + E_{R^+_{j,s}(D)}$.
- Return **Node**$(j, s,$ **BuildTree**$(R^-_{j,s}(D, k)),$ **BuildTree**$(R^+_{j,s}(D, k))$

Each call to **BuildTree** considers $O(dn)$ splits (for d dimensions, since we only need to split between each data point in each dimension); each requires $O(n)$ work where n is the number of data points considered ($n = |D|$ if all data points in D are used).

Study Question: Concretely, what would be a good set of split-points to consider for dimension j of a dataset D?

2.1.2 Pruning

It might be tempting to regularize by using a somewhat large value of k, or by stopping when splitting a node does not significantly decrease the error. One problem with short-sighted stopping criteria is that they might not see the value of a split that will require one more split before it seems useful.

Study Question: Apply the decision-tree algorithm to the XOR problem in two dimensions. What is the training-set error of all possible hypotheses based on a single split?

So, we will tend to build a tree that is too large, and then prune it back.

Define *cost complexity* of a tree T, where m ranges over its leaves as

$$C_\alpha(T) = \sum_{m=1}^{|T|} E_m(T) + \alpha|T| \quad .$$

and $|T|$ is the number of leaves. For a fixed α, we can find a T that (approximately) minimizes $C_\alpha(T)$ by "weakest-link" pruning:

- Create a sequence of trees by successively removing the bottom-level split that minimizes the increase in overall error, until the root is reached.
- Return the T in the sequence that minimizes the criterion.

We can choose an appropriate α using cross validation.

2.2 Classification

The strategy for building and pruning classification trees is very similar to the strategy for regression trees.

Given a region R_m corresponding to a leaf of the tree, we would pick the output class y to be the value that exists most frequently (the *majority value*) in the data points whose x values are in that region:

$$O_m = \text{majority}_{\{i|x^{(i)} \in R_m\}} y^{(i)} \quad .$$

Define the error in a region as the number of data points that do not have the value O_m:

$$E_m = \left|\{i \mid x^{(i)} \in R_m \text{ and } y^{(i)} \neq O_m\}\right| \quad .$$

Define the *empirical probability* of an item from class k occurring in region m as:

$$\hat{P}_{mk} = \hat{P}(R_m)(k) = \frac{\left|\{i \mid x^{(i)} \in R_m \text{ and } y^{(i)} = k\}\right|}{N_m} \quad ,$$

where N_m is the number of training points in region m. We'll define the empirical probabilities of split values, as well, for later use.

$$\hat{P}_{mjv} = \hat{P}(R_{mj})(v) = \frac{\left|\{i \mid x^{(i)} \in R_m \text{ and } x_j^{(i)} \geqslant v\}\right|}{N_m}$$

Splitting criteria In our greedy algorithm, we need a way to decide which split to make next. There are many criteria that express some measure of the "impurity" in child nodes. Some measures include:

- *Misclassification error*:
$$Q_m(T) = \frac{E_m}{N_m} = 1 - \hat{P}_{mO_m}$$
- *Gini index*:
$$Q_m(T) = \sum_k \hat{P}_{mk}(1 - \hat{P}_{mk})$$
- *Entropy*:
$$Q_m(T) = H(R_m) = -\sum_k \hat{P}_{mk} \log_2 \hat{P}_{mk}$$

So that this is well-defined when $\hat{P} = 0$, we will stipulate that $0 \log_2 0 = 0$.

They are very similar, and it's not entirely obvious which one is better. We will focus on entropy, just to be concrete.

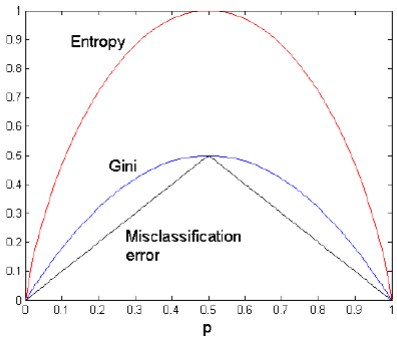
Choosing the split that minimizes the entropy of the children is equivalent to maximizing the *information gain* of the test $X_j = v$, defined by

$$\text{infoGain}(X_j = v, R_m) \quad = \quad H(R_m) - \left(\hat{P}_{mjv} H(R^+_{j,v}) + (1 - \hat{P}_{mjv}) H(R^-_{j,v})\right)$$

In the two-class case, all the criteria have the values

$$\begin{cases} 0.0 & \text{when } \hat{P}_{m0} = 0.0 \\ 0.0 & \text{when } \hat{P}_{m0} = 1.0 \end{cases}$$

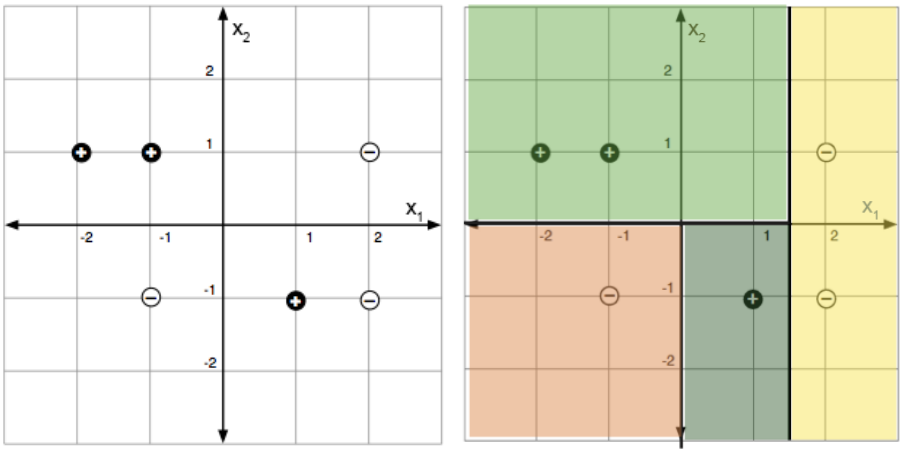
The respective impurity curves are shown below, where $p = \hat{p}_{m0}$:



There used to be endless haggling about which one to use. It seems to be traditional to use:

- Entropy to select which node to split while growing the tree
- Misclassification error in the pruning criterion

As a concrete example, consider the following images:



The left image depicts a set of labeled data points and the right shows a partition into regions by a decision tree.

Points about trees There are many variations on this theme:

- Linear regression or other regression or classification method in each leaf

- Non-axis-parallel splits: e.g., run a perceptron for a while to get a split.

What's good about trees:

- Easily interpretable
- Fast to train!
- Easy to handle multi-class classification
- Easy to handle different loss functions (just change predictor in the leaves)

What's bad about trees:

- High estimation error: small changes in the data can result in very big changes in the hypothesis.
- Often not the best predictions

Hierarchical mixture of experts Make a "soft" version of trees, in which the splits are probabilistic (so every point has some degree of membership in every leaf). Can be trained with a form of gradient descent.

3 Bagging

Bootstrap aggregation is a technique for reducing the estimation error of a non-linear predictor, or one that is adaptive to the data.

- Construct B new data sets of size n by sampling them with replacement from $\mathcal{D}$
- Train a predictor on each one: $\hat{f}^b$
- *Regression case*: bagged predictor is

$$\hat{f}_{bag}(x) = \frac{1}{B}\sum_{b=1}^{B} \hat{f}^b(x)$$

- *Classification case*: majority bagged predictor: let $\hat{f}^b(x)$ be a "one-hot" vector with a single 1 and $K-1$ zeros, so that $\hat{y}^b(x) = \arg\max_k \hat{f}^b(x)_k$. Then

$$\hat{f}_{bag}(x) = \frac{1}{B}\sum_{b=1}^{B} \hat{f}^b(x),$$

  which is a vector containing the proportion of classifiers that predicted each class k for input x; and the predicted output is

$$\hat{y}_{bag}(x) = \arg\max_k \hat{f}_{bag}(x)_k \quad .$$

There are theoretical arguments showing that bagging does, in fact, reduce estimation error. However, when we bag a model, any simple intrepetability is lost.

3.1 Random Forests

Random forests are collections of trees that are constructed to be de-correlated, so that using them to vote gives maximal advantage. In competitions, they often have the best classification performance among large collections of much fancier methods.

For $b = 1..B$

- Draw a bootstrap sample $\mathcal{D}_b$ of size n from $\mathcal{D}$
- Grow a tree on data $\mathcal{D}_b$ by recursively repeating these steps:
  - Select m variables at random from the d variables
  - Pick the best variable and split point among them
  - Split the node
- Return tree T_b

Given the ensemble of trees, vote to make a prediction on a new x.

4 Nearest Neighbor

In nearest-neighbor models, we don't do any processing of the data at training time – we just remember it! All the work is done at prediction time.

Input values x can be from any domain $\mathcal{X}$ ($\mathbb{R}^d$, documents, tree-structured objects, etc.). We just need a distance metric, $d : \mathcal{X} \times \mathcal{X} \to \mathbb{R}^+$, which satisfies the following, for all $x, x', x'' \in \mathcal{X}$:

$$\begin{aligned} d(x, x) &= 0 \\ d(x, x') &= d(x', x) \\ d(x, x'') &\leqslant d(x, x') + d(x', x'') \end{aligned}$$

Given a data-set $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^n$, our predictor for a new $x \in \mathcal{X}$ is

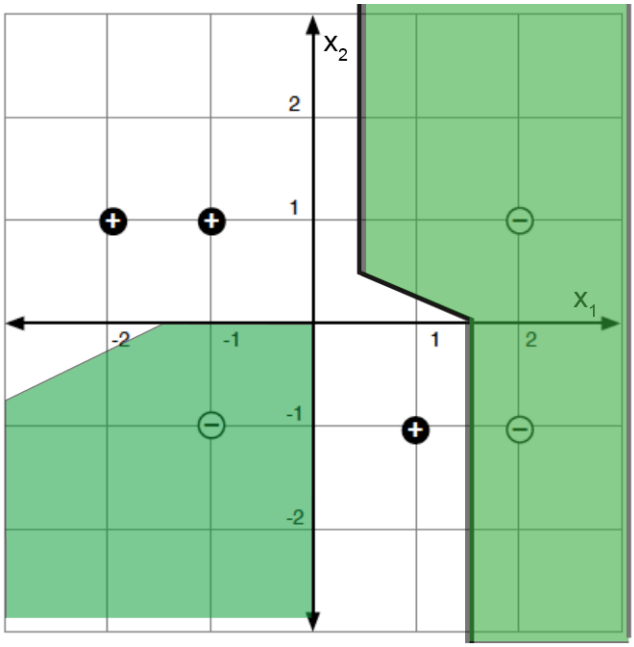
$$h(x) = y^{(i)} \quad \text{where} \quad i = \arg\min_i d(x, x^{(i)}) \ ,$$

that is, the predicted output associated with the training point that is closest to the query point x.

This same algorithm works for regression *and* classification!

It's a floor wax *and* a dessert topping!

The nearest neighbor prediction function can be described by a Voronoi partition (dividing the space up into regions whose closest point is each individual training point) as shown below:



In each region, we predict the associated y value.

Study Question: Convince yourself that these boundaries do represent the nearest-neighbor classifier derived from these 6 data points.

There are several useful variations on this method. In k-*nearest-neighbors*, we find the k training points nearest to the query point x and output the majority y value for classification or the average for regression. We can also do *locally weighted regression* in which we fit locally linear regression models to the k nearest points, possibly giving less weight to those that are farther away. In large data-sets, it is important to use good data structures (e.g., ball trees) to perform the nearest-neighbor look-ups efficiently (without looking at all the data points each time).

CHAPTER 14

Clustering

Oftentimes a dataset can be partitioned into different categories. A doctor may notice that their patients come in cohorts and different cohorts respond to different treatments. A biologist may gain insight by identifying that eagles and pigeons, despite outward appearances, have some underlying similarity, and both should be considered members of the same category, i.e., "bird". The problem of automatically identifying meaningful groupings in datasets is called clustering. Once these groupings are found, they can be leveraged toward interpreting the data and making optimal decisions for each group.

1 Clustering formalisms

Mathematically, clustering looks a bit like classification: we wish to find a mapping from datapoints, x, to categories, y. However, rather than the categories being predefined labels, the categories in clustering are automatically discovered *partitions* of an unlabeled dataset.

Because clustering does not learn from labeled examples, it is an example of an *unsupervised* learning algorithm. Instead of mimicking the mapping implicit in supervised training pairs $\{x^{(i)}, y^{(i)}\}_{i=1}^{n}$, clustering assigns datapoints to categories based on how the unlabeled data $\{x^{(i)}\}_{i=1}^{n}$ is *distributed* in data space.

Intuitively, a "cluster" is a groups of datapoints that are all nearby to each other and far away from other clusters. Let's consider the following scatter plot. How many clusters do you think there are?

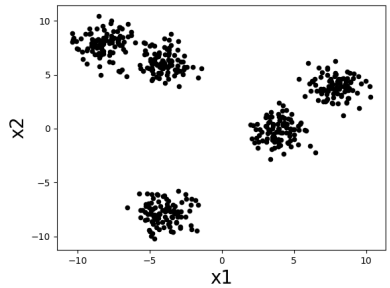


Figure 14.1: A dataset we would like to cluster. How many clusters do you think there are?

There seem to be about five clumps of datapoints and those clumps are what we would like to call clusters. If we assign all datapoints in each clump to a cluster corresponding to that clump then we have that nearby datapoints are assigned to the same cluster while far apart datapoints are assigned to different clusters, just what we wanted!

In designing clustering algorithms, three critical things we need to decide are:

- How do we measure *distance* between datapoints? What counts as "nearby" and "far apart"?
- How many clusters should we look for?
- How do we evaluate how good a clustering is?

We will see how to begin making these decisions as we work through a concrete clustering algorithm in the next section.

2 k-means

One of the simplest and most commonly used clustering algorithms is called k-means. The goal of the k-means algorithm is to assign datapoints to k clusters in such a way that the variance within clusters is as small as possible. Notice that this matches our intuitive idea that a cluster should be a tightly packed set of datapoints.

We will be careful to distinguish between the k-means *algorithm* and the k-means *objective*. As we will see, the k-means algorithm can be understood to be just one optimization algorithm which finds a local optima of the k-means objective.

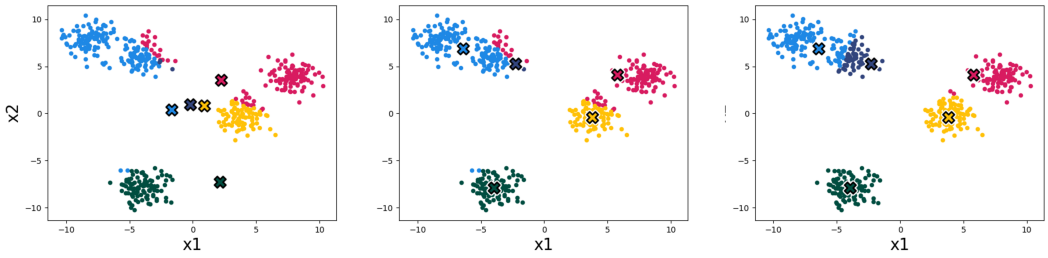
Similar to how we showed that supervised learning could be formalized mathematically as that of minimizing an objective function (loss function + regularization), we will show how unsupervised learning can also be formalized as minimizing an objective function. Let us denote the cluster assignment for a datapoint $x^{(i)}$ as $y^{(i)} \in \{1, 2, \ldots, k\}$, i.e., $y^{(i)} = 1$ means we are assigning datapoint $x^{(i)}$ to cluster number 1. Then the k-means objective can be quantified with the following objective function (which we also call the "k-means loss"):

$$\sum_{j=1}^{k} \sum_{i=1}^{n} 1(y^{(i)} = j) \left\| x^{(i)} - \mu^{(j)} \right\|_2^2 \tag{14.1}$$

Recall that *variance* is a measure of how "spread out" data is, defined as the mean squared distance from the average value of the data.

where $\mu^{(j)} = \frac{1}{N_j} \sum_{i=1}^{n} 1(y^{(i)} = j) x^{(i)}$, $N_j = \sum_{i=1}^{n} 1(y^{(i)} = j)$ (i.e., $\mu^{(j)}$ is the mean of all datapoints in cluster j), and $1(\cdot)$ is the indicator function (takes on value of 1 if its argument is true and 0 otherwise). The term inside the outer sum of the loss is the variance of datapoints within cluster j. We sum up the variance of all k clusters to get our overall loss.

The k-means algorithm minimizes this loss by alternating between two steps: given some initial cluster assignments, 1) compute the mean of all data in each cluster and assign this as the "cluster mean", 2) reassign each datapoint to the cluster with nearest cluster mean. Figure 14.2 shows what happens when we repeat these steps on the dataset from above.



1) Initial assignments 2) Update means 3) Update assignments

Figure 14.2: The first three steps of running k-means on this data. Datapoints are colored according to the cluster to which they are assigned. Cluster means are the larger X's with black outlines.

Each time we reassign the data to the nearest cluster mean, the k-means loss decreases (the datapoints end up closer to their assigned cluster mean), and each time we recompute the cluster means the loss *also* decreases (the means end up closer to their assigned datapoints). This leads to the clustering getting better and better with each iteration.

After four iterations of cluster assignment + update means, k-means converges to the solution shown in Figure 14.3.

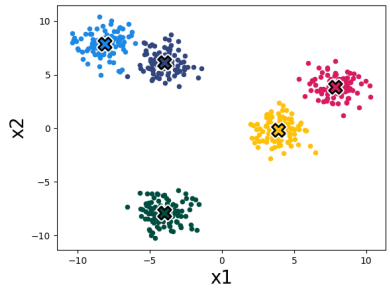


Figure 14.3: Converged result.

It seems to converge to something reasonable! Now let's write out the algorithm in complete detail:

K-MEANS$(k, \tau, \{x^{(i)}\}_{i=1}^{n})$

1 $\mu, y =$ randinit
2 **for** $t = 1$ **to** τ
3 $\quad y_{old} = y$
4 $\quad$ **for** $i = 1$ **to** n
5 $\quad\quad y^{(i)} = \arg\min_j \left\|x^{(i)} - \mu^{(j)}\right\|_2^2$
6 $\quad$ **for** $j = 1$ **to** k
7 $\quad\quad \mu^{(j)} = \frac{1}{N_j} \sum_{i=1}^{n} 1(y^{(i)} = j) x^{(i)}$
8 $\quad$ **if** $1(y = y_{old})$
9 $\quad\quad$ break
10 **return** μ, y

Study Question: Why do we have the "break" statement on line 9? Could the clustering improve if we ran it for more iterations after this point? Has it converged?

The for-loop over the n datapoints assigns each datapoint to the nearest cluster center. The for-loop over the k clusters updates the cluster center to be the mean of all datapoints currently assigned to that cluster. As suggested above, it can be shown that this algorithm reduces the loss in Eqn. 14.1 on each iteration, until it converges to a local minimum of the loss.

It's like classification except it *picked* what the classes are rather than being given examples of what the classes are.

2.1 Using gradient descent to minimize k-means objective

If that algorithm looked strange, don't worry, we can also just use gradient descent. To see how to apply gradient descent, we first rewrite the objective as a differentiable function *only of* μ:

$$L(\mu) = \sum_{i=1}^{n} \min_j \left\| x^{(i)} - \mu^{(j)} \right\|_2^2 \tag{14.2}$$

$L(\mu)$ is the value of the k-means loss given that we pick the *optimal* assignments of the datapoints to cluster means (that's what the $\min_j$ does). Now we can use the gradient $\frac{\partial L(\mu)}{\partial \mu}$ to find the values for μ that achieve minimum loss when cluster assignments are optimal. Finally, we read off the optimal cluster assignments, given the optimized μ, just by assigning datapoints to their nearest cluster mean:

$$y^{(i)} = \arg\min_j \left\| x^{(i)} - \mu^{(j)} \right\|_2^2 \tag{14.3}$$

This procedure yields a local minimum of Eqn. 14.1, just like the standard k-means algorithm we presented. It might not be the global optimum since the objective is not convex (due to $\min_j$: the minimum of multiple convex functions is not necessarily convex).

The k-means algorithm presented above is a form of *block coordinate descent*, rather than gradient descent. For certain problems, and in particular k-means, this method can converge faster than gradient descent.

$L(\mu)$ is a smooth function except with kinks where the nearest cluster changes; that means it's differentiable almost everywhere, which in practice is sufficient for us to apply gradient descent.

2.2 Importance of initialization

The standard k-means algorithm, as well as the variant that uses gradient descent, both are only guaranteed to converge to a local minimum, not necessarily the global minimum of the loss. Thus the answer we get out depends on how we initialize the cluster means. Here is an example of a different initialization on our toy data, which results in a worse converged clustering:

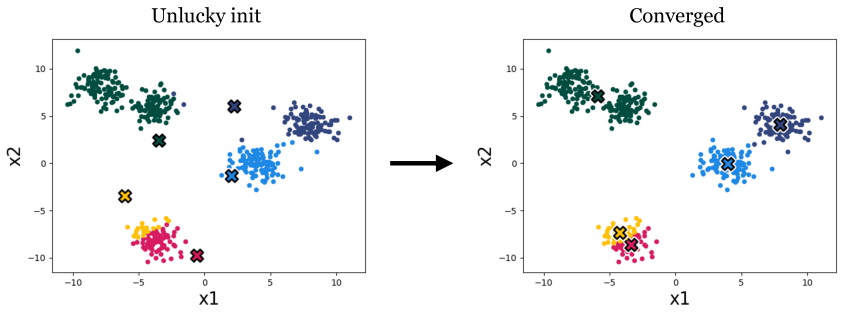


Figure 14.4: With the initialization of the means to the left, the yellow and red means end up splitting what perhaps should be one cluster in half.

A variety of methods have been developed to pick good initializations (see, for example, the *k-means++* algorithm). One simple option is to run the standard k-means algorithm

multiple times, with different random initial conditions, and then pick from these the clustering that achieves the lowest k-means loss.

2.3 Importance of k

A very important parameter in cluster algorithms is the number of clusters we are looking for. Some advanced algorithms can automatically infer a suitable number of clusters, but most of the time, like with k-means, we will have to pick k – it's a hyperparameter of the algorithm. Here's an example of the effect:

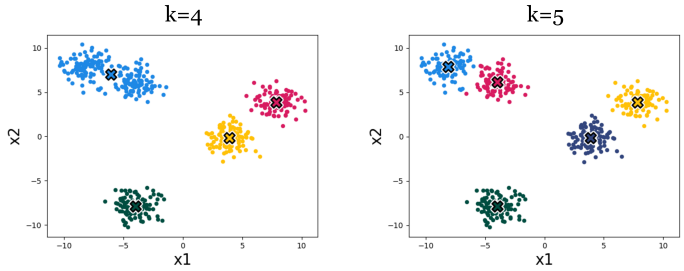


Figure 14.5: Example of k-means run on our toy data, with two different values of k. Setting k=4, on the left, results in one cluster being merged, compared to setting k=5, on the right. Which clustering do you think is better? How could you decide?

Which one looks more correct? It can be hard to say! Using higher k we get more clusters, and with more clusters we can achieve lower within-cluster variance – the k-means objective will typically decrease as we increase k. Eventually, we can increase k to equal the total number of datapoints, so that each datapoint is assigned to its own cluster. Then the k-means objective is zero, but the clustering reveals nothing. Clearly, then, we cannot use the k-means objective itself to choose the best value for k. In Section 3, we will discuss some ways of evaluating the success of clustering beyond its ability to minimize the k-means objective, and it's with these sorts of methods that we might decide on a proper value of k.

Alternatively, you may be wondering: why bother picking a single k? Wouldn't it be nice to reveal a *hierarchy* of clusterings of our data, showing both coarse and fine groupings? Indeed *hierarchical clustering* is another important class of clustering algorithms, beyond k-means. These methods can be useful for discovering tree-like structure in data, and they work a bit like the decision trees we saw in the last chapter, where initially a coarse split of the data is applied at the root of the tree, and then as we descend the tree we split the data in ever more fine-grained ways. A prototypical example of hierarchical clustering is to discover a taxonomy of life, where creatures may be grouped at multiple granularities, from species to families to kingdoms.

2.4 k-means in feature space

Clustering algorithms group data based on a notion of *similarity*. Thus we need to define a *distance metric* between datapoints, just like we did for nearest-neighbor methods. Here again our choice of metric has a big impact on the results we will find.

Our k-means algorithm uses the Euclidean distance, i.e., $\left\|x^{(i)} - \mu^{(j)}\right\|_2$, with a loss function that is the square of this distance. We can modify k-means to use different distance metrics, but a more common trick is to stick with Euclidean distance but measured in a *feature space*. Just like we did for regression and classification problems, we can define a

feature map from the data to a nicer feature representation, $\phi(x)$, and then apply k-means to cluster the data in the feature space.

As a simple example, suppose we have two-dimensional data that is very stretched out in the first dimension and has less dynamic range in the second dimension. Then we may want to scale the dimensions so that each has similar dynamic range, prior to clustering. We could use standardization, like we did in Chapter 4.

If we want to cluster more complex data, like images, music, chemical compounds, etc., then we will usually need more sophisticated feature representations. One common practice these days is to use feature representations learned with a neural network. For example, we can use an autoencoder to compress images into feature vectors, then cluster those feature vectors.

In fact, using a simple distance metric in feature space can be equivalent to using a more sophisticated distance metric in the data space, and this trick forms the basis of *kernel methods*, which you can learn about in more advanced machine learning classes.

3 How to evaluate clustering algorithms

One of the hardest aspects of clustering is knowing how to evaluate it. This is actually a big issue for all unsupervised learning methods, since we are just looking for patterns in the data, rather than explicitly trying to predict target values (which was the case with supervised learning).

Remember, evaluation metrics are *not* the same as loss functions, so we can't just measure success by looking at the k-means loss. In prediction problems, it is critical that the evaluation is on a held-out test set, while the loss is computed over training data. If we evaluate on training data we cannot detect overfitting. Something similar is going on with the example in Section 2.3, where setting k to be too large can precisely "fit" the data (minimize the loss), but yields no general insight.

One way to evaluate our clusters is to look at the **consistency** with which they are found when we run on different subsamples of our training data, or with different hyperparameters of our clustering algorithm (e.g., initializations). For example, if running on several bootstrapped samples results in very different clusters, it should call into question the validity of any of the individual results.

If we have some notion of what **ground truth** clusters should be, e.g., a few data points that we know should be in the same cluster, then we can measure whether or not our discovered clusters group these examples correctly.

Clustering is often used for **visualization** and **interpretability**, to make it easier for humans to understand the data. Here, human judgment may guide the choice of clustering algorithm.

More quantitatively, discovered clusters may be used as input to **downstream tasks**. For example, we may fit a different regression function on the data within each cluster. Figure 14.6, on the following page, gives an example where this might be useful.

In cases like this, the success of a clustering algorithm can be indirectly measured based on the success of the downstream application (e.g., does it make the downstream predictions more accurate).

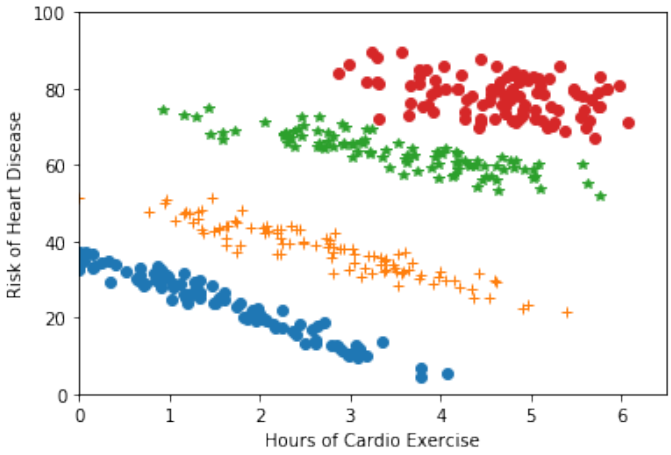


Figure 14.6: Averaged across the whole population, risk of heart disease positively correlates with hours of exercise. However, if we cluster the data, we can observe that there are four subgroups of the population, which correspond to different age groups, and within each subgroup the correlation is negative. We can make better predictions, and better capture the presumed true effect, if we cluster this data and then model the trend in each cluster separately.

CHAPTER 15

Appendices

1 Unsupervised learning with autoencoders

So far we have studied learning to predict labels, such as for classification or regression. What if you do not have labels? As introduced in Section 1.2, another type of machine learning, *unsupervised learning*, can be used to discover patterns in data when you don't have labels. Some examples of this are to discover and characterize underlying factors of variation in data, which can aid in scientific discovery, to compress data for efficient storage or communication, or to use as a pre-processing step prior to supervised learning, reducing the amount of data that is needed to learn a good classifier or regressor.

Autoencoders are a family of unsupervised learning algorithms that obtain these insights by seeking to learn compressed versions of the original data. Assume that we have input data $\mathcal{D} = \{x^{(1)}, \ldots, x^{(n)}\}$, where $x^{(i)} \in \mathbb{R}^d$. The algorithms will output a new dataset $\mathcal{D}_{\text{out}} = \{a^{(1)}, \ldots, a^{(n)}\}$, where $a^{(i)} \in \mathbb{R}^k$ with $k < d$. We can think about $a^{(i)}$ as the new *representation* of data point $x^{(i)}$. For example, in Fig. 15.1 we show the learned representations of a dataset of MNIST digits with $k = 2$. We see, after inspecting the individual data points, unsupervised learning has automatically grouped together images of the same digit.

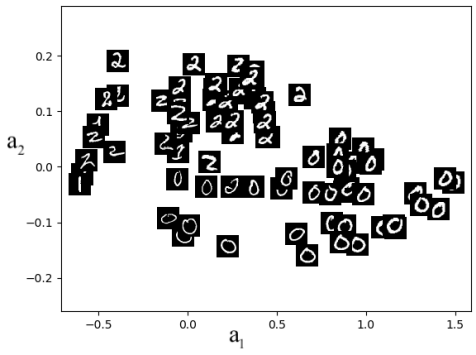


Figure 15.1: Compression of digits dataset into two dimensions. The input $x^{(i)}$, an image of a handwritten digit, is shown at the new low-dimensional representation (a_1, a_2).

Formally, an autoencoder consists of two functions, a vector-valued *encoder* $g : \mathbb{R}^d \to \mathbb{R}^k$ which deterministically maps the data to the representation space $a \in \mathbb{R}^k$ and a *decoder* $h : \mathbb{R}^k \to \mathbb{R}^d$ which maps the representation space back into the original data space. The basic architecture of an autoencoder is shown in Figure 15.2. In this example, the original d-dimensional input is compressed into $k = 3$ dimensions via the encoder $g(x; W^1) = f_1(W^{1T} x)$ with $W^1 \in \mathbb{R}^{d \times k}$ (the non-linearity f_1 is applied to each dimension of the vector). To recover (an approximation to) the original instance, we then apply the decoder $h(a; W^2) = f_2(W^{2T} a)$, where f_2 denotes a different non-linearity (activation function). In general, both the decoder and the encoder could involve multiple layers, as opposed to the single layer shown here. Learning seeks parameters W^1 and W^2 such that the reconstructed instances, $h(g(x^{(i)}; W^1); W^2)$, are close to the original input $x^{(i)}$.

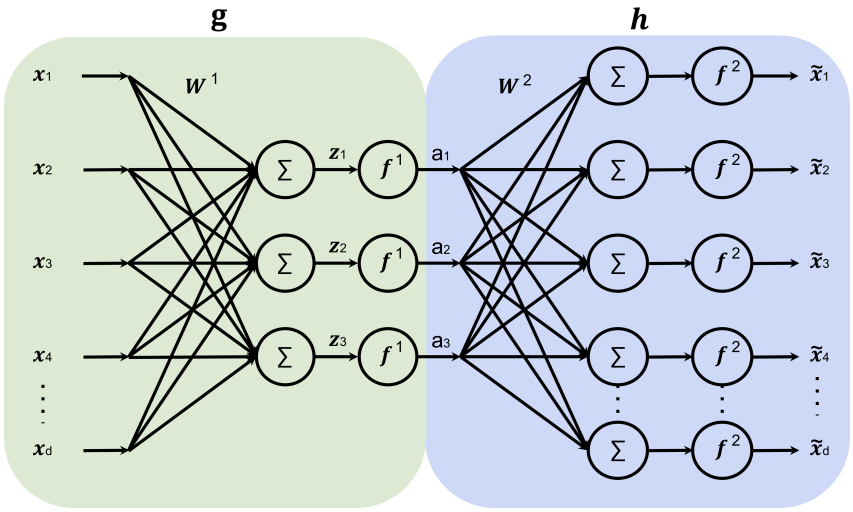


Figure 15.2: Autoencoder structure, showing the encoder (left half, light green), and the decoder (right half, light blue), encoding inputs x to the representation a, and decoding the representation to produce $\tilde{x}$, the reconstruction. In this specific example, the representation (a_1, a_2, a_3) only has three dimensions.

We learn autoencoders using the same tools we previously used for supervised learning, namely (stochastic) gradient descent of a multi-layer neural network to minimize a loss function. All that remains is to specify the loss function $L(\tilde{x}, x)$, which tells us how to measure the discrepancy between the reconstruction $\tilde{x} = h(g(x; W^1); W^2)$ and the original input x. For example, for continuous-valued x it might make sense to use squared loss, i.e. $L(\tilde{x}, x) = \sum_{j=1}^{d} (x_j - \tilde{x}_j)^2$. Learning then seeks to optimize the parameters of h and g so as to minimize the reconstruction error, measured according to this loss function:

$$\min_{W^1, W^2} \sum_{i=1}^{n} L\left(h(g(x^{(i)}; W^1); W^2), x^{(i)}\right)$$

Alternatively, you could think of this as *multi-task learning*, where the goal is to predict each dimension of x. One can mix-and-match loss functions as appropriate for each dimension's data type.

What makes a good representation? Notice that, without further constraints, it is always possible to perfectly reconstruct the input. For example, we could let $k = d$ and h and g be the identity functions. In this case, we would not obtain any compression of the data. To learn something useful, we must create a *bottleneck* by making k to be much smaller than d. This forces the learning algorithm to seek transformations that describe the original data using as simple a description as possible. Thinking back to the digits dataset, for example, an example of a compressed representation might be the digit label (i.e., 0–9), rotation, and stroke thickness. Of course, there is no guarantee that the learning algorithm

will discover precisely this representation. After learning, we can inspect the learned representations, such as by artificially increasing or decreasing one of the dimensions (e.g. a_1) and seeing how it affects the output $h(a)$, to try to better understand what it has learned.

We close by mentioning that even linear encoders and decoders can be very powerful. In this case, rather than minimizing the above objective with gradient descent, a technique called *principal components analysis* can be used to obtain a closed-form solution to the optimization problem using a singular value decomposition. More broadly, there are many types of unsupervised learning. Later in the semester we will learn about *clustering*, where $k = 1$ and a_i takes a discrete number indicating the cluster in which each data point is assigned.