Chapter 2

Linear Algebra

Linear algebra is a branch of mathematics that is widely used throughout science and engineering. However, because linear algebra is a form of continuous rather than discrete mathematics, many computer scientists have little experience with it. A good understanding of linear algebra is essential for understanding and working with many machine learning algorithms, especially deep learning algorithms. We therefore precede our introduction to deep learning with a focused presentation of the key linear algebra prerequisites.

If you are already familiar with linear algebra, feel free to skip this chapter. If you have previous experience with these concepts but need a detailed reference sheet to review key formulas, we recommend *The Matrix Cookbook* (Petersen and Pedersen, 2006). If you have no exposure at all to linear algebra, this chapter will teach you enough to read this book, but we highly recommend that you also consult another resource focused exclusively on teaching linear algebra, such as Shilov (1977). This chapter will completely omit many important linear algebra topics that are not essential for understanding deep learning.

2.1 Scalars, Vectors, Matrices and Tensors

The study of linear algebra involves several types of mathematical objects:

- *Scalars*: A scalar is just a single number, in contrast to most of the other objects studied in linear algebra, which are usually arrays of multiple numbers. We write scalars in italics. We usually give scalars lower-case variable names. When we introduce them, we specify what kind of number they are. For

example, we might say "Let $s \in \mathbb{R}$ be the slope of the line," while defining a real-valued scalar, or "Let $n \in \mathbb{N}$ be the number of units," while defining a natural number scalar.

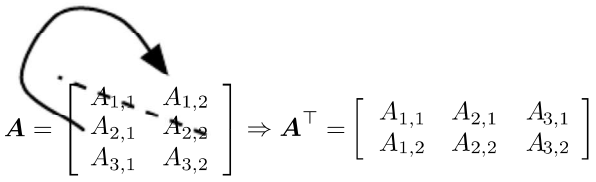
- *Vectors*: A vector is an array of numbers. The numbers are arranged in order. We can identify each individual number by its index in that ordering. Typically we give vectors lower case names written in bold typeface, such as $\boldsymbol{x}$. The elements of the vector are identified by writing its name in italic typeface, with a subscript. The first element of $\boldsymbol{x}$ is x_1, the second element is x_2 and so on. We also need to say what kind of numbers are stored in the vector. If each element is in $\mathbb{R}$, and the vector has n elements, then the vector lies in the set formed by taking the Cartesian product of $\mathbb{R}$ n times, denoted as $\mathbb{R}^n$. When we need to explicitly identify the elements of a vector, we write them as a column enclosed in square brackets:

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}. \tag{2.1}$$

  We can think of vectors as identifying points in space, with each element giving the coordinate along a different axis.

  Sometimes we need to index a set of elements of a vector. In this case, we define a set containing the indices and write the set as a subscript. For example, to access x_1, x_3 and x_6, we define the set $S = \{1, 3, 6\}$ and write $\boldsymbol{x}_S$. We use the $-$ sign to index the complement of a set. For example $\boldsymbol{x}_{-1}$ is the vector containing all elements of $\boldsymbol{x}$ except for x_1, and $\boldsymbol{x}_{-S}$ is the vector containing all of the elements of $\boldsymbol{x}$ except for x_1, x_3 and x_6.

- *Matrices*: A matrix is a 2-D array of numbers, so each element is identified by two indices instead of just one. We usually give matrices upper-case variable names with bold typeface, such as $\boldsymbol{A}$. If a real-valued matrix $\boldsymbol{A}$ has a height of m and a width of n, then we say that $\boldsymbol{A} \in \mathbb{R}^{m \times n}$. We usually identify the elements of a matrix using its name in italic but not bold font, and the indices are listed with separating commas. For example, $A_{1,1}$ is the upper left entry of $\boldsymbol{A}$ and $A_{m,n}$ is the bottom right entry. We can identify all of the numbers with vertical coordinate i by writing a ":" for the horizontal coordinate. For example, $\boldsymbol{A}_{i,:}$ denotes the horizontal cross section of $\boldsymbol{A}$ with vertical coordinate i. This is known as the i-th *row* of $\boldsymbol{A}$. Likewise, $\boldsymbol{A}_{:,i}$ is



$$\boldsymbol{A} = \begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \\ A_{3,1} & A_{3,2} \end{bmatrix} \Rightarrow \boldsymbol{A}^\top = \begin{bmatrix} A_{1,1} & A_{2,1} & A_{3,1} \\ A_{1,2} & A_{2,2} & A_{3,2} \end{bmatrix}$$

Figure 2.1: The transpose of the matrix can be thought of as a mirror image across the main diagonal.

the i-th *column* of $\boldsymbol{A}$. When we need to explicitly identify the elements of a matrix, we write them as an array enclosed in square brackets:

$$\begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{bmatrix}. \tag{2.2}$$

Sometimes we may need to index matrix-valued expressions that are not just a single letter. In this case, we use subscripts after the expression, but do not convert anything to lower case. For example, $f(\boldsymbol{A})_{i,j}$ gives element (i, j) of the matrix computed by applying the function f to $\boldsymbol{A}$.

- *Tensors*: In some cases we will need an array with more than two axes. In the general case, an array of numbers arranged on a regular grid with a variable number of axes is known as a *tensor*. We denote a tensor named "A" with this typeface: A. We identify the element of A at coordinates (i, j, k) by writing $\mathsf{A}_{i,j,k}$.

One important operation on matrices is the *transpose*. The transpose of a matrix is the mirror image of the matrix across a diagonal line, called the *main diagonal*, running down and to the right, starting from its upper left corner. See Fig. 2.1 for a graphical depiction of this operation. We denote the transpose of a matrix $\boldsymbol{A}$ as $\boldsymbol{A}^\top$, and it is defined such that

$$(\boldsymbol{A}^\top)_{i,j} = A_{j,i}. \tag{2.3}$$

Vectors can be thought of as matrices that contain only one column. The transpose of a vector is therefore a matrix with only one row. Sometimes we

define a vector by writing out its elements in the text inline as a row matrix, then using the transpose operator to turn it into a standard column vector, e.g., $\boldsymbol{x} = [x_1, x_2, x_3]^\top$.

A scalar can be thought of as a matrix with only a single entry. From this, we can see that a scalar is its own transpose: $a = a^\top$.

We can add matrices to each other, as long as they have the same shape, just by adding their corresponding elements: $\boldsymbol{C} = \boldsymbol{A} + \boldsymbol{B}$ where $C_{i,j} = A_{i,j} + B_{i,j}$.

We can also add a scalar to a matrix or multiply a matrix by a scalar, just by performing that operation on each element of a matrix: $\boldsymbol{D} = a \cdot \boldsymbol{B} + c$ where $D_{i,j} = a \cdot B_{i,j} + c$.

In the context of deep learning, we also use some less conventional notation. We allow the addition of matrix and a vector, yielding another matrix: $\boldsymbol{C} = \boldsymbol{A} + \boldsymbol{b}$, where $C_{i,j} = A_{i,j} + b_j$. In other words, the vector $\boldsymbol{b}$ is added to each row of the matrix. This shorthand eliminates the need to define a matrix with $\boldsymbol{b}$ copied into each row before doing the addition. This implicit copying of $\boldsymbol{b}$ to many locations is called *broadcasting*.

2.2 Multiplying Matrices and Vectors

One of the most important operations involving matrices is multiplication of two matrices. The *matrix product* of matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ is a third matrix $\boldsymbol{C}$. In order for this product to be defined, $\boldsymbol{A}$ must have the same number of columns as $\boldsymbol{B}$ has rows. If $\boldsymbol{A}$ is of shape $m \times n$ and $\boldsymbol{B}$ is of shape $n \times p$, then $\boldsymbol{C}$ is of shape $m \times p$. We can write the matrix product just by placing two or more matrices together, e.g.

$$\boldsymbol{C} = \boldsymbol{A}\boldsymbol{B}. \tag{2.4}$$

The product operation is defined by

$$C_{i,j} = \sum_k A_{i,k} B_{k,j}. \tag{2.5}$$

Note that the standard product of two matrices is *not* just a matrix containing the product of the individual elements. Such an operation exists and is called the *element-wise product* or *Hadamard product*, and is denoted as $\boldsymbol{A} \odot \boldsymbol{B}$.

The *dot product* between two vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ of the same dimensionality is the matrix product $\boldsymbol{x}^\top \boldsymbol{y}$. We can think of the matrix product $\boldsymbol{C} = \boldsymbol{A}\boldsymbol{B}$ as computing $C_{i,j}$ as the dot product between row i of $\boldsymbol{A}$ and column j of $\boldsymbol{B}$.

Matrix product operations have many useful properties that make mathematical analysis of matrices more convenient. For example, matrix multiplication is distributive:

$$\boldsymbol{A}(\boldsymbol{B} + \boldsymbol{C}) = \boldsymbol{A}\boldsymbol{B} + \boldsymbol{A}\boldsymbol{C}. \tag{2.6}$$

It is also associative:

$$\boldsymbol{A}(\boldsymbol{B}\boldsymbol{C}) = (\boldsymbol{A}\boldsymbol{B})\boldsymbol{C}. \tag{2.7}$$

Matrix multiplication is *not* commutative (the condition $\boldsymbol{A}\boldsymbol{B} = \boldsymbol{B}\boldsymbol{A}$ does not always hold), unlike scalar multiplication. However, the dot product between two vectors is commutative:

$$\boldsymbol{x}^\top \boldsymbol{y} = \boldsymbol{y}^\top \boldsymbol{x}. \tag{2.8}$$

The transpose of a matrix product has a simple form:

$$(\boldsymbol{A}\boldsymbol{B})^\top = \boldsymbol{B}^\top \boldsymbol{A}^\top. \tag{2.9}$$

This allows us to demonstrate Eq. 2.8, by exploiting the fact that the value of such a product is a scalar and therefore equal to its own transpose:

$$\boldsymbol{x}^\top \boldsymbol{y} = \left(\boldsymbol{x}^\top \boldsymbol{y}\right)^\top = \boldsymbol{y}^\top \boldsymbol{x}. \tag{2.10}$$

Since the focus of this textbook is not linear algebra, we do not attempt to develop a comprehensive list of useful properties of the matrix product here, but the reader should be aware that many more exist.

We now know enough linear algebra notation to write down a system of linear equations:

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b} \tag{2.11}$$

where $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ is a known matrix, $\boldsymbol{b} \in \mathbb{R}^m$ is a known vector, and $\boldsymbol{x} \in \mathbb{R}^n$ is a vector of unknown variables we would like to solve for. Each element x_i of $\boldsymbol{x}$ is one of these unknown variables. Each row of $\boldsymbol{A}$ and each element of $\boldsymbol{b}$ provide another constraint. We can rewrite Eq. 2.11 as:

$$\boldsymbol{A}_{1,:}\, \boldsymbol{x} = b_1 \tag{2.12}$$

$$\boldsymbol{A}_{2,:}\, \boldsymbol{x} = b_2 \tag{2.13}$$

$$\dots \tag{2.14}$$

$$\boldsymbol{A}_{m,:}\, \boldsymbol{x} = b_m \tag{2.15}$$

or, even more explicitly, as:

$$\boldsymbol{A}_{1,1} x_1 + \boldsymbol{A}_{1,2} x_2 + \cdots + \boldsymbol{A}_{1,n} x_n = b_1 \tag{2.16}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Figure 2.2: *Example identity matrix*: This is $\boldsymbol{I}_3$.

$$\boldsymbol{A}_{2,1}x_1 + \boldsymbol{A}_{2,2}x_2 + \cdots + \boldsymbol{A}_{2,n}x_n = b_2 \tag{2.17}$$

$$\cdots \tag{2.18}$$

$$\boldsymbol{A}_{m,1}x_1 + \boldsymbol{A}_{m,2}x_2 + \cdots + \boldsymbol{A}_{m,n}x_n = b_m\,. \tag{2.19}$$

Matrix-vector product notation provides a more compact representation for equations of this form.

2.3 Identity and Inverse Matrices

Linear algebra offers a powerful tool called *matrix inversion* that allows us to analytically solve Eq. 2.11 for many values of $\boldsymbol{A}$.

To describe matrix inversion, we first need to define the concept of an *identity matrix*. An identity matrix is a matrix that does not change any vector when we multiply that vector by that matrix. We denote the identity matrix that preserves n-dimensional vectors as $\boldsymbol{I}_n$. Formally, $\boldsymbol{I}_n \in \mathbb{R}^{n\times n}$, and

$$\forall \boldsymbol{x} \in \mathbb{R}^n, \boldsymbol{I}_n\boldsymbol{x} = \boldsymbol{x}. \tag{2.20}$$

The structure of the identity matrix is simple: all of the entries along the main diagonal are 1, while all of the other entries are zero. See Fig. 2.2 for an example.

The *matrix inverse* of $\boldsymbol{A}$ is denoted as $\boldsymbol{A}^{-1}$, and it is defined as the matrix such that

$$\boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{I}_n\,. \tag{2.21}$$

We can now solve Eq. 2.11 by the following steps:

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b} \tag{2.22}$$

$$\boldsymbol{A}^{-1}\boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b} \tag{2.23}$$

$$\boldsymbol{I}_n\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b} \tag{2.24}$$

$$\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}. \tag{2.25}$$

Of course, this depends on it being possible to find $\boldsymbol{A}^{-1}$. We discuss the conditions for the existence of $\boldsymbol{A}^{-1}$ in the following section.

When $\boldsymbol{A}^{-1}$ exists, several different algorithms exist for finding it in closed form. In theory, the same inverse matrix can then be used to solve the equation many times for different values of $\boldsymbol{b}$. However, $\boldsymbol{A}^{-1}$ is primarily useful as a theoretical tool, and should not actually be used in practice for most software applications. Because $\boldsymbol{A}^{-1}$ can be represented with only limited precision on a digital computer, algorithms that make use of the value of $\boldsymbol{b}$ can usually obtain more accurate estimates of $\boldsymbol{x}$.

2.4 Linear Dependence and Span

In order for $\boldsymbol{A}^{-1}$ to exist, Eq. 2.11 must have exactly one solution for every value of $\boldsymbol{b}$. However, it is also possible for the system of equations to have no solutions or infinitely many solutions for some values of $\boldsymbol{b}$. It is not possible to have more than one but less than infinitely many solutions for a particular $\boldsymbol{b}$; if both $\boldsymbol{x}$ and $\boldsymbol{y}$ are solutions then

$$\boldsymbol{z} = \alpha\boldsymbol{x} + (1 - \alpha)\boldsymbol{y} \tag{2.26}$$

is also a solution for any real α.

To analyze how many solutions the equation has, we can think of the columns of $\boldsymbol{A}$ as specifying different directions we can travel from the *origin* (the point specified by the vector of all zeros), and determine how many ways there are of reaching $\boldsymbol{b}$. In this view, each element of $\boldsymbol{x}$ specifies how far we should travel in each of these directions, with x_i specifying how far to move in the direction of column i:

$$\boldsymbol{A}\boldsymbol{x} = \sum_i x_i \boldsymbol{A}_{:,i}. \tag{2.27}$$

In general, this kind of operation is called a *linear combination*. Formally, a linear combination of some set of vectors $\{\boldsymbol{v}^{(1)}, \ldots, \boldsymbol{v}^{(n)}\}$ is given by multiplying each vector $\boldsymbol{v}^{(i)}$ by a corresponding scalar coefficient and adding the results:

$$\sum_i c_i \boldsymbol{v}^{(i)}. \tag{2.28}$$

The *span* of a set of vectors is the set of all points obtainable by linear combination of the original vectors.

Determining whether $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ has a solution thus amounts to testing whether $\boldsymbol{b}$ is in the span of the columns of $\boldsymbol{A}$. This particular span is known as the *column space* or the *range* of $\boldsymbol{A}$.

In order for the system $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ to have a solution for all values of $\boldsymbol{b} \in \mathbb{R}^m$, we therefore require that the column space of $\boldsymbol{A}$ be all of $\mathbb{R}^m$. If any point in $\mathbb{R}^m$ is excluded from the column space, that point is a potential value of $\boldsymbol{b}$ that has no solution. The requirement that the column space of $\boldsymbol{A}$ be all of $\mathbb{R}^m$ implies immediately that $\boldsymbol{A}$ must have at least m columns, i.e., $n \geq m$. Otherwise, the dimensionality of the column space would be less than m. For example, consider a 3×2 matrix. The target $\boldsymbol{b}$ is 3-D, but $\boldsymbol{x}$ is only 2-D, so modifying the value of $\boldsymbol{x}$ at best allows us to trace out a 2-D plane within $\mathbb{R}^3$. The equation has a solution if and only if $\boldsymbol{b}$ lies on that plane.

Having $n \geq m$ is only a necessary condition for every point to have a solution. It is not a sufficient condition, because it is possible for some of the columns to be redundant. Consider a 2×2 matrix where both of the columns are identical. This has the same column space as a 2×1 matrix containing only one copy of the replicated column. In other words, the column space is still just a line, and fails to encompass all of $\mathbb{R}^2$, even though there are two columns.

Formally, this kind of redundancy is known as *linear dependence*. A set of vectors is *linearly independent* if no vector in the set is a linear combination of the other vectors. If we add a vector to a set that is a linear combination of the other vectors in the set, the new vector does not add any points to the set's span. This means that for the column space of the matrix to encompass all of $\mathbb{R}^m$, the matrix must contain at least one set of m linearly independent columns. This condition is both necessary and sufficient for Eq. 2.11 to have a solution for every value of $\boldsymbol{b}$. Note that the requirement is for a set to have exactly m linear independent columns, not at least m. No set of m-dimensional vectors can have more than m mutually linearly independent columns, but a matrix with more than m columns may have more than one such set.

In order for the matrix to have an inverse, we additionally need to ensure that Eq. 2.11 has *at most* one solution for each value of $\boldsymbol{b}$. To do so, we need to ensure that the matrix has at most m columns. Otherwise there is more than one way of parametrizing each solution.

Together, this means that the matrix must be *square*, that is, we require that $m = n$ and that all of the columns must be linearly independent. A square matrix with linearly dependent columns is known as *singular*.

If $\boldsymbol{A}$ is not square or is square but singular, it can still be possible to solve the

equation. However, we can not use the method of matrix inversion to find the solution.

So far we have discussed matrix inverses as being multiplied on the left. It is also possible to define an inverse that is multiplied on the right:

$$\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{I}. \tag{2.29}$$

For square matrices, the left inverse and right inverse are equal.

2.5 Norms

Sometimes we need to measure the size of a vector. In machine learning, we usually measure the size of vectors using a function called a *norm*. Formally, the L^p norm is given by

$$||\boldsymbol{x}||_p = \left(\sum_i |x_i|^p\right)^{\frac{1}{p}} \tag{2.30}$$

for $p \in \mathbb{R}, p \geq 1$.

Norms, including the L^p norm, are functions mapping vectors to non-negative values. On an intuitive level, the norm of a vector $\boldsymbol{x}$ measures the distance from the origin to the point $\boldsymbol{x}$. More rigorously, a norm is any function f that satisfies the following properties:

- $f(\boldsymbol{x}) = 0 \Rightarrow \boldsymbol{x} = \boldsymbol{0}$
- $f(\boldsymbol{x} + \boldsymbol{y}) \leq f(\boldsymbol{x}) + f(\boldsymbol{y})$ (the *triangle inequality*)
- $\forall \alpha \in \mathbb{R}, f(\alpha\boldsymbol{x}) = |\alpha| f(\boldsymbol{x})$

The L^2 norm, with $p = 2$, is known as the *Euclidean norm*. It is simply the Euclidean distance from the origin to the point identified by $\boldsymbol{x}$. The L^2 norm is used so frequently in machine learning that it is often denoted simply as $||\boldsymbol{x}||$, with the subscript 2 omitted. It is also common to measure the size of a vector using the squared L^2 norm, which can be calculated simply as $\boldsymbol{x}^\top\boldsymbol{x}$.

The squared L^2 norm is more convenient to work with mathematically and computationally than the L^2 norm itself. For example, the derivatives of the squared L^2 norm with respect to each element of $\boldsymbol{x}$ each depend only on the corresponding element of $\boldsymbol{x}$, while all of the derivatives of the L^2 norm depend on the entire vector. In many contexts, the squared L^2 norm may be undesirable

because it increases very slowly near the origin. In several machine learning applications, it is important to discriminate between elements that are exactly zero and elements that are small but nonzero. In these cases, we turn to a function that grows at the same rate in all locations, but retains mathematical simplicity: the L^1 norm. The L^1 norm may be simplified to

$$||\boldsymbol{x}||_1 = \sum_i |x_i|. \tag{2.31}$$

The L^1 norm is commonly used in machine learning when the difference between zero and nonzero elements is very important. Every time an element of $\boldsymbol{x}$ moves away from 0 by ϵ, the L^1 norm increases by ϵ.

We sometimes measure the size of the vector by counting its number of nonzero elements. Some authors refer to this function as the "L^0 norm," but this is incorrect terminology. The number of non-zero entries in a vector is not a norm, because scaling the vector by α does not change the number of nonzero entries. The L^1 norm is often used as a substitute for the number of nonzero entries.

One other norm that commonly arises in machine learning is the L^∞ norm, also known as the *max norm*. This norm simplifies to the absolute value of the element with the largest magnitude in the vector,

$$||\boldsymbol{x}||_\infty = \max_i |x_i|. \tag{2.32}$$

Sometimes we may also wish to measure the size of a matrix. In the context of deep learning, the most common way to do this is with the otherwise obscure *Frobenius norm*

$$||A||_F = \sqrt{\sum_{i,j} A_{i,j}^2}, \tag{2.33}$$

which is analogous to the L^2 norm of a vector.

The dot product of two vectors can be rewritten in terms of norms. Specifically,

$$\boldsymbol{x}^\top \boldsymbol{y} = ||\boldsymbol{x}||_2 ||\boldsymbol{y}||_2 \cos\theta \tag{2.34}$$

where θ is the angle between $\boldsymbol{x}$ and $\boldsymbol{y}$.

2.6 Special Kinds of Matrices and Vectors

Some special kinds of matrices and vectors are particularly useful.

Diagonal matrices consist mostly of zeros and have non-zero entries only along the main diagonal. Formally, a matrix $\boldsymbol{D}$ is diagonal if and only if $D_{i,j} = 0$ for all $i \neq j$. We have already seen one example of a diagonal matrix: the identity matrix, where all of the diagonal entries are 1. We write $\text{diag}(\boldsymbol{v})$ to denote a square diagonal matrix whose diagonal entries are given by the entries of the vector $\boldsymbol{v}$. Diagonal matrices are of interest in part because multiplying by a diagonal matrix is very computationally efficient. To compute $\text{diag}(\boldsymbol{v})\boldsymbol{x}$, we only need to scale each element x_i by v_i. In other words, $\text{diag}(\boldsymbol{v})\boldsymbol{x} = \boldsymbol{v} \odot \boldsymbol{x}$. Inverting a square diagonal matrix is also efficient. The inverse exists only if every diagonal entry is nonzero, and in that case, $\text{diag}(\boldsymbol{v})^{-1} = \text{diag}([1/v_1, \ldots, 1/v_n]^\top)$. In many cases, we may derive some very general machine learning algorithm in terms of arbitrary matrices, but obtain a less expensive (and less descriptive) algorithm by restricting some matrices to be diagonal.

Not all diagonal matrices need be square. It is possible to construct a rectangular diagonal matrix. Non-square diagonal matrices do not have inverses but it is still possible to multiply by them cheaply. For a non-square diagonal matrix $\boldsymbol{D}$, the product $\boldsymbol{Dx}$ will involve scaling each element of $\boldsymbol{x}$, and either concatenating some zeros to the result if $\boldsymbol{D}$ is taller than it is wide, or discarding some of the last elements of the vector if $\boldsymbol{D}$ is wider than it is tall.

A *symmetric* matrix is any matrix that is equal to its own transpose:

$$\boldsymbol{A} = \boldsymbol{A}^\top. \tag{2.35}$$

Symmetric matrices often arise when the entries are generated by some function of two arguments that does not depend on the order of the arguments. For example, if $\boldsymbol{A}$ is a matrix of distance measurements, with $\boldsymbol{A}_{i,j}$ giving the distance from point i to point j, then $\boldsymbol{A}_{i,j} = \boldsymbol{A}_{j,i}$ because distance functions are symmetric.

A *unit vector* is a vector with *unit norm*:

$$||\boldsymbol{x}||_2 = 1. \tag{2.36}$$

A vector $\boldsymbol{x}$ and a vector $\boldsymbol{y}$ are *orthogonal* to each other if $\boldsymbol{x}^\top \boldsymbol{y} = 0$. If both vectors have nonzero norm, this means that they are at a 90 degree angle to each other. In $\mathbb{R}^n$, at most n vectors may be mutually orthogonal with nonzero norm. If the vectors are not only orthogonal but also have unit norm, we call them *orthonormal*.

An *orthogonal matrix* is a square matrix whose rows are mutually orthonormal and whose columns are mutually orthonormal:

$$\boldsymbol{A}^\top \boldsymbol{A} = \boldsymbol{A}\boldsymbol{A}^\top = \boldsymbol{I}. \tag{2.37}$$

This implies that

$$\boldsymbol{A}^{-1} = \boldsymbol{A}^\top, \tag{2.38}$$

so orthogonal matrices are of interest because their inverse is very cheap to compute. Pay careful attention to the definition of orthogonal matrices. Counterintuitively, their rows are not merely orthogonal but fully orthonormal. There is no special term for a matrix whose rows or columns are orthogonal but not orthonormal.

2.7 Eigendecomposition

Many mathematical objects can be understood better by breaking them into constituent parts, or finding some properties of them that are universal, not caused by the way we choose to represent them.

For example, integers can be decomposed into prime factors. The way we represent the number 12 will change depending on whether we write it in base ten or in binary, but it will always be true that $12 = 2 \times 2 \times 3$. From this representation we can conclude useful properties, such as that 12 is not divisible by 5, or that any integer multiple of 12 will be divisible by 3.

Much as we can discover something about the true nature of an integer by decomposing it into prime factors, we can also decompose matrices in ways that show us information about their functional properties that is not obvious from the representation of the matrix as an array of elements.

One of the most widely used kinds of matrix decomposition is called *eigendecomposition*, in which we decompose a matrix into a set of eigenvectors and eigenvalues.

An *eigenvector* of a square matrix $\boldsymbol{A}$ is a non-zero vector $\boldsymbol{v}$ such that multiplication by $\boldsymbol{A}$ alters only the scale of $\boldsymbol{v}$:

$$\boldsymbol{A}\boldsymbol{v} = \lambda \boldsymbol{v}. \tag{2.39}$$

The scalar λ is known as the *eigenvalue* corresponding to this eigenvector. (One can also find a *left eigenvector* such that $\boldsymbol{v}^\top \boldsymbol{A} = \lambda \boldsymbol{v}^\top$, but we are usually concerned with right eigenvectors).

If $\boldsymbol{v}$ is an eigenvector of $\boldsymbol{A}$, then so is any rescaled vector $s\boldsymbol{v}$ for $s \in \mathbb{R}, s \neq 0$. Moreover, $s\boldsymbol{v}$ still has the same eigenvalue. For this reason, we usually only look for unit eigenvectors.

Suppose that a matrix $\boldsymbol{A}$ has n linearly independent eigenvectors, $\{\boldsymbol{v}^{(1)}, \ldots, \boldsymbol{v}^{(n)}\}$, with corresponding eigenvalues $\{\lambda_1, \ldots, \lambda_n\}$. We may concatenate all of the

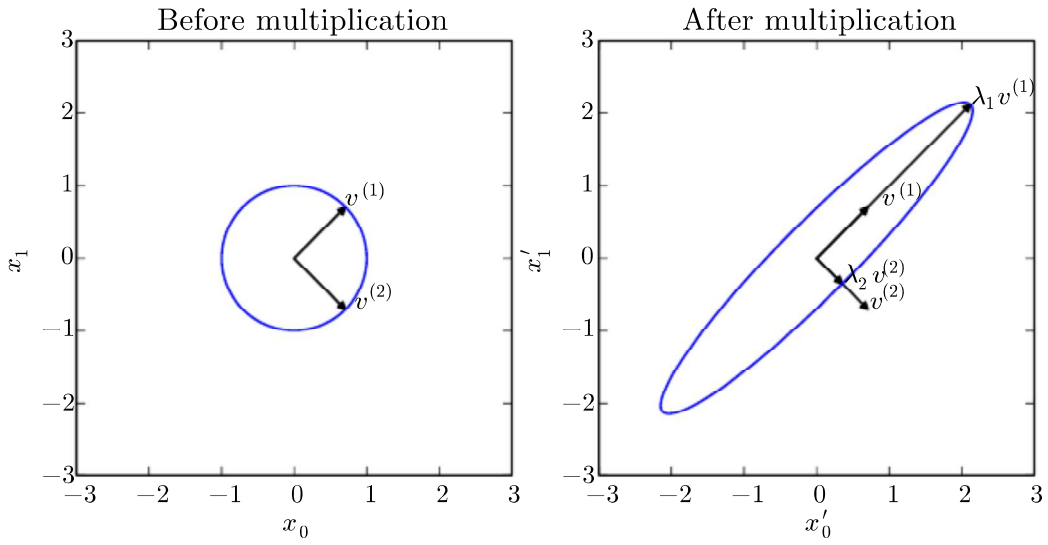


Figure 2.3: An example of the effect of eigenvectors and eigenvalues. Here, we have a matrix $\boldsymbol{A}$ with two orthonormal eigenvectors, $\boldsymbol{v}^{(1)}$ with eigenvalue λ_1 and $\boldsymbol{v}^{(2)}$ with eigenvalue λ_2. *(Left)* We plot the set of all unit vectors $\boldsymbol{u} \in \mathbb{R}^2$ as a unit circle. *(Right)* We plot the set of all points $\boldsymbol{Au}$. By observing the way that $\boldsymbol{A}$ distorts the unit circle, we can see that it scales space in direction $\boldsymbol{v}^{(i)}$ by λ_i.

eigenvectors to form a matrix $\boldsymbol{V}$ with one eigenvector per column: $\boldsymbol{V} = [\boldsymbol{v}^{(1)}, \ldots, \boldsymbol{v}^{(n)}]$. Likewise, we can concatenate the eigenvalues to form a vector $\boldsymbol{\lambda} = [\lambda_1, \ldots, \lambda_n]^\top$. The *eigendecomposition* of $\boldsymbol{A}$ is then given by

$$\boldsymbol{A} = \boldsymbol{V}\text{diag}(\boldsymbol{\lambda})\boldsymbol{V}^{-1}. \tag{2.40}$$

We have seen that *constructing* matrices with specific eigenvalues and eigenvectors allows us to stretch space in desired directions. However, we often want to *decompose* matrices into their eigenvalues and eigenvectors. Doing so can help us to analyze certain properties of the matrix, much as decomposing an integer into its prime factors can help us understand the behavior of that integer.

Not every matrix can be decomposed into eigenvalues and eigenvectors. In some

cases, the decomposition exists, but may involve complex rather than real numbers. Fortunately, in this book, we usually need to decompose only a specific class of matrices that have a simple decomposition. Specifically, every real symmetric matrix can be decomposed into an expression using only real-valued eigenvectors and eigenvalues:

$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^\top, \tag{2.41}$$

where $\boldsymbol{Q}$ is an orthogonal matrix composed of eigenvectors of $\boldsymbol{A}$, and $\boldsymbol{\Lambda}$ is a diagonal matrix. The eigenvalue $\Lambda_{i,i}$ is associated with the eigenvector in column i of $\boldsymbol{Q}$, denoted as $\boldsymbol{Q}_{:,i}$. Because $\boldsymbol{Q}$ is an orthogonal matrix, we can think of $\boldsymbol{A}$ as scaling space by λ_i in direction $\boldsymbol{v}^{(i)}$. See Fig. 2.3 for an example.

While any real symmetric matrix $\boldsymbol{A}$ is guaranteed to have an eigendecomposition, the eigendecomposition may not be unique. If any two or more eigenvectors share the same eigenvalue, then any set of orthogonal vectors lying in their span are also eigenvectors with that eigenvalue, and we could equivalently choose a $\boldsymbol{Q}$ using those eigenvectors instead. By convention, we usually sort the entries of $\boldsymbol{\Lambda}$ in descending order. Under this convention, the eigendecomposition is unique only if all of the eigenvalues are unique.

The eigendecomposition of a matrix tells us many useful facts about the matrix. The matrix is singular if and only if any of the eigenvalues are zero. The eigendecomposition of a real symmetric matrix can also be used to optimize quadratic expressions of the form $f(\boldsymbol{x}) = \boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x}$ subject to $||\boldsymbol{x}||_2 = 1$. Whenever $\boldsymbol{x}$ is equal to an eigenvector of $\boldsymbol{A}$, f takes on the value of the corresponding eigenvalue. The maximum value of f within the constraint region is the maximum eigenvalue and its minimum value within the constraint region is the minimum eigenvalue.

A matrix whose eigenvalues are all positive is called *positive definite*. A matrix whose eigenvalues are all positive or zero-valued is called *positive semidefinite*. Likewise, if all eigenvalues are negative, the matrix is *negative definite*, and if all eigenvalues are negative or zero-valued, it is *negative semidefinite*. Positive semidefinite matrices are interesting because they guarantee that $\forall \boldsymbol{x},\ \boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} \geq 0$. Positive definite matrices additionally guarantee that $\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} = 0 \Rightarrow \boldsymbol{x} = \boldsymbol{0}$.

2.8 Singular Value Decomposition

In Sec. 2.7, we saw how to decompose a matrix into eigenvectors and eigenvalues. The *singular value decomposition* (SVD) provides another way to factorize a matrix, into *singular vectors* and *singular values*. The SVD allows us to discover some of the same kind of information as the eigendecomposition. However, the SVD is

more generally applicable. Every real matrix has a singular value decomposition, but the same is not true of the eigenvalue decomposition. For example, if a matrix is not square, the eigendecomposition is not defined, and we must use a singular value decomposition instead.

Recall that the eigendecomposition involves analyzing a matrix $\boldsymbol{A}$ to discover a matrix $\boldsymbol{V}$ of eigenvectors and a vector of eigenvalues $\boldsymbol{\lambda}$ such that we can rewrite $\boldsymbol{A}$ as

$$\boldsymbol{A} = \boldsymbol{V}\text{diag}(\boldsymbol{\lambda})\boldsymbol{V}^{-1}. \tag{2.42}$$

The singular value decomposition is similar, except this time we will write $\boldsymbol{A}$ as a product of three matrices:

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^{\top}. \tag{2.43}$$

Suppose that $\boldsymbol{A}$ is an $m \times n$ matrix. Then $\boldsymbol{U}$ is defined to be an $m \times m$ matrix, $\boldsymbol{D}$ to be an $m \times n$ matrix, and $\boldsymbol{V}$ to be an $n \times n$ matrix.

Each of these matrices is defined to have a special structure. The matrices $\boldsymbol{U}$ and $\boldsymbol{V}$ are both defined to be orthogonal matrices. The matrix $\boldsymbol{D}$ is defined to be a diagonal matrix. Note that $\boldsymbol{D}$ is not necessarily square.

The elements along the diagonal of $\boldsymbol{D}$ are known as the *singular values* of the matrix $\boldsymbol{A}$. The columns of $\boldsymbol{U}$ are known as the *left-singular vectors*. The columns of $\boldsymbol{V}$ are known as as the *right-singular vectors*.

We can actually interpret the singular value decomposition of $\boldsymbol{A}$ in terms of the eigendecomposition of functions of $\boldsymbol{A}$. The left-singular vectors of $\boldsymbol{A}$ are the eigenvectors of $\boldsymbol{A}\boldsymbol{A}^{\top}$. The right-singular vectors of $\boldsymbol{A}$ are the eigenvectors of $\boldsymbol{A}^{\top}\boldsymbol{A}$. The non-zero singular values of $\boldsymbol{A}$ are the square roots of the eigenvalues of $\boldsymbol{A}^{\top}\boldsymbol{A}$. The same is true for $\boldsymbol{A}\boldsymbol{A}^{\top}$.

Perhaps the most useful feature of the SVD is that we can use it to partially generalize matrix inversion to non-square matrices, as we will see in the next section.

2.9 The Moore-Penrose Pseudoinverse

Matrix inversion is not defined for matrices that are not square. Suppose we want to make a left-inverse $\boldsymbol{B}$ of a matrix $\boldsymbol{A}$, so that we can solve a linear equation

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{y} \tag{2.44}$$

by left-multiplying each side to obtain

$$\boldsymbol{x} = \boldsymbol{B}\boldsymbol{y}. \tag{2.45}$$

Depending on the structure of the problem, it may not be possible to design a unique mapping from $\boldsymbol{A}$ to $\boldsymbol{B}$.

If $\boldsymbol{A}$ is taller than it is wide, then it is possible for this equation to have no solution. If $\boldsymbol{A}$ is wider than it is tall, then there could be multiple possible solutions.

The *Moore-Penrose pseudoinverse* allows us to make some headway in these cases. The pseudoinverse of $\boldsymbol{A}$ is defined as a matrix

$$\boldsymbol{A}^+ = \lim_{\alpha \searrow 0} (\boldsymbol{A}^\top \boldsymbol{A} + \alpha \boldsymbol{I})^{-1} \boldsymbol{A}^\top. \tag{2.46}$$

Practical algorithms for computing the pseudoinverse are not based on this definition, but rather the formula

$$\boldsymbol{A}^+ = \boldsymbol{V}\boldsymbol{D}^+\boldsymbol{U}^\top, \tag{2.47}$$

where $\boldsymbol{U}$, $\boldsymbol{D}$ and $\boldsymbol{V}$ are the singular value decomposition of $\boldsymbol{A}$, and the pseudoinverse $\boldsymbol{D}^+$ of a diagonal matrix $\boldsymbol{D}$ is obtained by taking the reciprocal of its non-zero elements then taking the transpose of the resulting matrix.

When $\boldsymbol{A}$ has more columns than rows, then solving a linear equation using the pseudoinverse provides one of the many possible solutions. Specifically, it provides the solution $\boldsymbol{x} = \boldsymbol{A}^+\boldsymbol{y}$ with minimal Euclidean norm $||\boldsymbol{x}||_2$ among all possible solutions.

When $\boldsymbol{A}$ has more rows than columns, it is possible for there to be no solution. In this case, using the pseudoinverse gives us the $\boldsymbol{x}$ for which $\boldsymbol{A}\boldsymbol{x}$ is as close as possible to $\boldsymbol{y}$ in terms of Euclidean norm $||\boldsymbol{A}\boldsymbol{x} - \boldsymbol{y}||_2$.

2.10 The Trace Operator

The trace operator gives the sum of all of the diagonal entries of a matrix:

$$\mathrm{Tr}(\boldsymbol{A}) = \sum_i \boldsymbol{A}_{i,i}. \tag{2.48}$$

The trace operator is useful for a variety of reasons. Some operations that are difficult to specify without resorting to summation notation can be specified using

matrix products and the trace operator. For example, the trace operator provides an alternative way of writing the Frobenius norm of a matrix:

$$||A||_F = \sqrt{\text{Tr}(\boldsymbol{A}\boldsymbol{A}^\top)}. \tag{2.49}$$

Writing an expression in terms of the trace operator opens up opportunities to manipulate the expression using many useful identities. For example, the trace operator is invariant to the transpose operator:

$$\text{Tr}(\boldsymbol{A}) = \text{Tr}(\boldsymbol{A}^\top). \tag{2.50}$$

The trace of a square matrix composed of many factors is also invariant to moving the last factor into the first position, if the shapes of the corresponding matrices allow the resulting product to be defined:

$$\text{Tr}(\boldsymbol{A}\boldsymbol{B}\boldsymbol{C}) = \text{Tr}(\boldsymbol{C}\boldsymbol{A}\boldsymbol{B}) = \text{Tr}(\boldsymbol{B}\boldsymbol{C}\boldsymbol{A}) \tag{2.51}$$

or more generally,

$$\text{Tr}(\prod_{i=1}^{n} \boldsymbol{F}^{(i)}) = \text{Tr}(\boldsymbol{F}^{(n)} \prod_{i=1}^{n-1} \boldsymbol{F}^{(i)}). \tag{2.52}$$

This invariance to cyclic permutation holds even if the resulting product has a different shape. For example, for $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ and $\boldsymbol{B} \in \mathbb{R}^{n \times m}$, we have

$$\text{Tr}(\boldsymbol{A}\boldsymbol{B}) = \text{Tr}(\boldsymbol{B}\boldsymbol{A}) \tag{2.53}$$

even though $\boldsymbol{A}\boldsymbol{B} \in \mathbb{R}^{m \times m}$ and $\boldsymbol{B}\boldsymbol{A} \in \mathbb{R}^{n \times n}$.

Another useful fact to keep in mind is that a scalar is its own trace: $a = \text{Tr}(a)$.

2.11 The Determinant

The determinant of a square matrix, denoted $\det(\boldsymbol{A})$, is a function mapping matrices to real scalars. The determinant is equal to the product of all the eigenvalues of the matrix. The absolute value of the determinant can be thought of as a measure of how much multiplication by the matrix expands or contracts space. If the determinant is 0, then space is contracted completely along at least one dimension, causing it to lose all of its volume. If the determinant is 1, then the transformation is volume-preserving.

2.12 Example: Principal Components Analysis

One simple machine learning algorithm, *principal components analysis* or *PCA* can be derived using only knowledge of basic linear algebra.

Suppose we have a collection of m points $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ in $\mathbb{R}^n$. Suppose we would like to apply lossy compression to these points. Lossy compression means storing the points in a way that requires less memory but may lose some precision. We would like to lose as little precision as possible.

One way we can encode these points is to represent a lower-dimensional version of them. For each point $\boldsymbol{x}^{(i)} \in \mathbb{R}^n$ we will find a corresponding code vector $\boldsymbol{c}^{(i)} \in \mathbb{R}^l$. If l is smaller than n, it will take less memory to store the code points than the original data. We will want to find some encoding function that produces the code for an input, $f(\boldsymbol{x}) = \boldsymbol{c}$, and a decoding function that produces the reconstructed input given its code, $\boldsymbol{x} \approx g(f(\boldsymbol{x}))$.

PCA is defined by our choice of the decoding function. Specifically, to make the decoder very simple, we choose to use matrix multiplication to map the code back into $\mathbb{R}^n$. Let $g(\boldsymbol{c}) = \boldsymbol{D}\boldsymbol{c}$, where $\boldsymbol{D} \in \mathbb{R}^{n \times l}$ is the matrix defining the decoding.

Computing the optimal code for this decoder could be a difficult problem. To keep the encoding problem easy, PCA constrains the columns of $\boldsymbol{D}$ to be orthogonal to each other. (Note that $\boldsymbol{D}$ is still not technically "an orthogonal matrix" unless $l = n$)

With the problem as described so far, many solutions are possible, because we can increase the scale of $\boldsymbol{D}_{:,i}$ if we decrease c_i proportionally for all points. To give the problem a unique solution, we constrain all of the columns of $\boldsymbol{D}$ to have unit norm.

In order to turn this basic idea into an algorithm we can implement, the first thing we need to do is figure out how to generate the optimal code point $\boldsymbol{c}^*$ for each input point $\boldsymbol{x}$. One way to do this is to minimize the distance between the input point $\boldsymbol{x}$ and its reconstruction, $g(\boldsymbol{c}^*)$. We can measure this distance using a norm. In the principal components algorithm, we use the L^2 norm:

$$\boldsymbol{c}^* = \arg\min_{\boldsymbol{c}} ||\boldsymbol{x} - g(\boldsymbol{c})||_2. \tag{2.54}$$

We can switch to the squared L^2 norm instead of the L^2 norm itself, because both are minimized by the same value of $\boldsymbol{c}$. This is because the L^2 norm is non-negative and the squaring operation is monotonically increasing for non-negative

arguments.

$$\boldsymbol{c}^* = \arg\min_{\boldsymbol{c}} ||\boldsymbol{x} - g(\boldsymbol{c})||_2^2. \tag{2.55}$$

The function being minimized simplifies to

$$(\boldsymbol{x} - g(\boldsymbol{c}))^\top (\boldsymbol{x} - g(\boldsymbol{c})) \tag{2.56}$$

(by the definition of the L^2 norm, Eq. 2.30)

$$= \boldsymbol{x}^\top \boldsymbol{x} - \boldsymbol{x}^\top g(\boldsymbol{c}) - g(\boldsymbol{c})^\top \boldsymbol{x} + g(\boldsymbol{c})^\top g(\boldsymbol{c}) \tag{2.57}$$

(by the distributive property)

$$= \boldsymbol{x}^\top \boldsymbol{x} - 2\boldsymbol{x}^\top g(\boldsymbol{c}) + g(\boldsymbol{c})^\top g(\boldsymbol{c}) \tag{2.58}$$

(because the scalar $g(\boldsymbol{x})^\top \boldsymbol{x}$ is equal to the transpose of itself).

We can now change the function being minimized again, to omit the first term, since this term does not depend on $\boldsymbol{c}$:

$$\boldsymbol{c}^* = \arg\min_{\boldsymbol{c}} -2\boldsymbol{x}^\top g(\boldsymbol{c}) + g(\boldsymbol{c})^\top g(\boldsymbol{c}). \tag{2.59}$$

To make further progress, we must substitute in the definition of $g(\boldsymbol{c})$:

$$\boldsymbol{c}^* = \arg\min_{\boldsymbol{c}} -2\boldsymbol{x}^\top \boldsymbol{D}\boldsymbol{c} + \boldsymbol{c}^\top \boldsymbol{D}^\top \boldsymbol{D}\boldsymbol{c} \tag{2.60}$$

$$= \arg\min_{\boldsymbol{c}} -2\boldsymbol{x}^\top \boldsymbol{D}\boldsymbol{c} + \boldsymbol{c}^\top \boldsymbol{I}_l \boldsymbol{c} \tag{2.61}$$

(by the orthogonality and unit norm constraints on $\boldsymbol{D}$)

$$= \arg\min_{\boldsymbol{c}} -2\boldsymbol{x}^\top \boldsymbol{D}\boldsymbol{c} + \boldsymbol{c}^\top \boldsymbol{c} \tag{2.62}$$

We can solve this optimization problem using vector calculus (see Sec. 4.3 if you do not know how to do this):

$$\nabla_{\boldsymbol{c}}(-2\boldsymbol{x}^\top \boldsymbol{D}\boldsymbol{c} + \boldsymbol{c}^\top \boldsymbol{c}) = \boldsymbol{0} \tag{2.63}$$

$$-2\boldsymbol{D}^\top \boldsymbol{x} + 2\boldsymbol{c} = \boldsymbol{0} \tag{2.64}$$

$$\boldsymbol{c} = \boldsymbol{D}^\top \boldsymbol{x}. \tag{2.65}$$

This makes the algorithm efficient: we can optimally encode $\boldsymbol{x}$ just using a matrix-vector operation. To encode a vector, we apply the encoder function

$$f(\boldsymbol{x}) = \boldsymbol{D}^\top \boldsymbol{x}. \tag{2.66}$$

Using a further matrix multiplication, we can also define the PCA reconstruction operation:

$$r(\boldsymbol{x}) = g\left(f\left(\boldsymbol{x}\right)\right) = \boldsymbol{D}\boldsymbol{D}^{\top}\boldsymbol{x}. \tag{2.67}$$

Next, we need to choose the encoding matrix $\boldsymbol{D}$. To do so, we revisit the idea of minimizing the L^2 distance between inputs and reconstructions. However, since we will use the same matrix $\boldsymbol{D}$ to decode all of the points, we can no longer consider the points in isolation. Instead, we must minimize the Frobenius norm of the matrix of errors computed over all dimensions and all points:

$$\boldsymbol{D}^{*} = \arg\min_{\boldsymbol{D}} \sqrt{\sum_{i,j}\left(x_j^{(i)} - r(\boldsymbol{x}^{(i)})_j\right)^2} \text{ subject to } \boldsymbol{D}^{\top}\boldsymbol{D} = \boldsymbol{I}_l \tag{2.68}$$

To derive the algorithm for finding $\boldsymbol{D}^{*}$, we will start by considering the case where $l = 1$. In this case, $\boldsymbol{D}$ is just a single vector, $\boldsymbol{d}$. Substituting Eq. 2.67 into Eq. 2.68 and simplifying $\boldsymbol{D}$ into $\boldsymbol{d}$, the problem reduces to

$$\boldsymbol{d}^{*} = \arg\min_{\boldsymbol{d}} \sum_i ||\boldsymbol{x}^{(i)} - \boldsymbol{d}\boldsymbol{d}^{\top}\boldsymbol{x}^{(i)}||_2^2 \text{ subject to } ||\boldsymbol{d}||_2 = 1. \tag{2.69}$$

The above formulation is the most direct way of performing the substitution, but is not the most stylistically pleasing way to write the equation. It places the scalar value $\boldsymbol{d}^{\top}\boldsymbol{x}^{(i)}$ on the right of the vector $\boldsymbol{d}$. It is more conventional to write scalar coefficients on the left of vector they operate on. We therefore usually write such a formula as

$$\boldsymbol{d}^{*} = \arg\min_{\boldsymbol{d}} \sum_i ||\boldsymbol{x}^{(i)} - \boldsymbol{d}^{\top}\boldsymbol{x}^{(i)}\boldsymbol{d}||_2^2 \text{ subject to } ||\boldsymbol{d}||_2 = 1, \tag{2.70}$$

or, exploiting the fact that a scalar is its own transpose, as

$$\boldsymbol{d}^{*} = \arg\min_{\boldsymbol{d}} \sum_i ||\boldsymbol{x}^{(i)} - \boldsymbol{x}^{(i)\top}\boldsymbol{d}\boldsymbol{d}||_2^2 \text{ subject to } ||\boldsymbol{d}||_2 = 1. \tag{2.71}$$

The reader should aim to become familiar with such cosmetic rearrangements.

At this point, it can be helpful to rewrite the problem in terms of a single design matrix of examples, rather than as a sum over separate example vectors. This will allow us to use more compact notation. Let $\boldsymbol{X} \in \mathbb{R}^{m\times n}$ be the matrix defined by stacking all of the vectors describing the points, such that $\boldsymbol{X}_{i,:} = \boldsymbol{x}^{(i)\top}$. We can now rewrite the problem as

$$\boldsymbol{d}^{*} = \arg\min_{\boldsymbol{d}} ||\boldsymbol{X} - \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^{\top}||_F^2 \text{ subject to } \boldsymbol{d}^{\top}\boldsymbol{d} = 1. \tag{2.72}$$

Disregarding the constraint for the moment, we can simplify the Frobenius norm portion as follows:

$$\arg\min_{\boldsymbol{d}} ||\boldsymbol{X} - \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top||_F^2 \tag{2.73}$$

$$= \arg\min_{\boldsymbol{d}} \operatorname{Tr}\left(\left(\boldsymbol{X} - \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top\right)^\top \left(\boldsymbol{X} - \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top\right)\right) \tag{2.74}$$

(by Eq. 2.49)

$$= \arg\min_{\boldsymbol{d}} \operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X} - \boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top - \boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X} + \boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) \tag{2.75}$$

$$= \arg\min_{\boldsymbol{d}} \operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}) - \operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) - \operatorname{Tr}(\boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X}) + \operatorname{Tr}(\boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) \tag{2.76}$$

$$= \arg\min_{\boldsymbol{d}} -\operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) - \operatorname{Tr}(\boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X}) + \operatorname{Tr}(\boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) \tag{2.77}$$

(because terms not involving $\boldsymbol{d}$ do not affect the arg min)

$$= \arg\min_{\boldsymbol{d}} -2\operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) + \operatorname{Tr}(\boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) \tag{2.78}$$

(because we can cycle the order of the matrices inside a trace, Eq. 2.52)

$$= \arg\min_{\boldsymbol{d}} -2\operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) + \operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{d}\boldsymbol{d}^\top) \tag{2.79}$$

(using the same property again)

At this point, we re-introduce the constraint:

$$\arg\min_{\boldsymbol{d}} -2\operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) + \operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top\boldsymbol{d} = 1 \tag{2.80}$$

$$= \arg\min_{\boldsymbol{d}} -2\operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) + \operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top\boldsymbol{d} = 1 \tag{2.81}$$

(due to the constraint)

$$= \arg\min_{\boldsymbol{d}} -\operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top\boldsymbol{d} = 1 \tag{2.82}$$

$$= \arg\max_{\boldsymbol{d}} \operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top\boldsymbol{d} = 1 \tag{2.83}$$

$$= \arg\max_{\boldsymbol{d}} \operatorname{Tr}(\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}) \text{ subject to } \boldsymbol{d}^\top\boldsymbol{d} = 1 \tag{2.84}$$

This optimization problem may be solved using eigendecomposition. Specifically, the optimal $\boldsymbol{d}$ is given by the eigenvector of $\boldsymbol{X}^\top \boldsymbol{X}$ corresponding to the largest eigenvalue.

In the general case, where $l > 1$, the matrix $\boldsymbol{D}$ is given by the l eigenvectors corresponding to the largest eigenvalues. This may be shown using proof by induction. We recommend writing this proof as an exercise.

Linear algebra is one of the fundamental mathematical disciplines that is necessary to understand deep learning. Another key area of mathematics that is ubiquitous in machine learning is probability theory, presented next.

Chapter 3

Probability and Information Theory

In this chapter, we describe probability theory and information theory.

Probability theory is a mathematical framework for representing uncertain statements. It provides a means of quantifying uncertainty and axioms for deriving new uncertain statements. In artificial intelligence applications, we use probability theory in two major ways. First, the laws of probability tell us how AI systems should reason, so we design our algorithms to compute or approximate various expressions derived using probability theory. Second, we can use probability and statistics to theoretically analyze the behavior of proposed AI systems.

Probability theory is a fundamental tool of many disciplines of science and engineering. We provide this chapter to ensure that readers whose background is primarily in software engineering with limited exposure to probability theory can understand the material in this book.

While probability theory allows us to make uncertain statements and reason in the presence of uncertainty, information allows us to quantify the amount of uncertainty in a probability distribution.

If you are already familiar with probability theory and information theory, you may wish to skip all of this chapter except for Sec. 3.14, which describes the graphs we use to describe structured probabilistic models for machine learning. If you have absolutely no prior experience with these subjects, this chapter should be sufficient to successfully carry out deep learning research projects, but we do suggest that you consult an additional resource, such as Jaynes (2003).

3.1 Why Probability?

Many branches of computer science deal mostly with entities that are entirely deterministic and certain. A programmer can usually safely assume that a CPU will execute each machine instruction flawlessly. Errors in hardware do occur, but are rare enough that most software applications do not need to be designed to account for them. Given that many computer scientists and software engineers work in a relatively clean and certain environment, it can be surprising that machine learning makes heavy use of probability theory.

This is because machine learning must always deal with uncertain quantities, and sometimes may also need to deal with stochastic (non-deterministic) quantities. Uncertainty and stochasticity can arise from many sources. Researchers have made compelling arguments for quantifying uncertainty using probability since at least the 1980s. Many of the arguments presented here are summarized from or inspired by Pearl (1988).

Nearly all activities require some ability to reason in the presence of uncertainty. In fact, beyond mathematical statements that are true by definition, it is difficult to think of any proposition that is absolutely true or any event that is absolutely guaranteed to occur.

There are three possible sources of uncertainty:

1. Inherent stochasticity in the system being modeled. For example, most interpretations of quantum mechanics describe the dynamics of subatomic particles as being probabilistic. We can also create theoretical scenarios that we postulate to have random dynamics, such as a hypothetical card game where we assume that the cards are truly shuffled into a random order.

2. Incomplete observability. Even deterministic systems can appear stochastic when we cannot observe all of the variables that drive the behavior of the system. For example, in the Monty Hall problem, a game show contestant is asked to choose between three doors and wins a prize held behind the chosen door. Two doors lead to a goat while a third leads to a car. The outcome given the contestant's choice is deterministic, but from the contestant's point of view, the outcome is uncertain.

3. Incomplete modeling. When we use a model that must discard some of the information we have observed, the discarded information results in uncertainty in the model's predictions. For example, suppose we build a robot that can exactly observe the location of every object around it. If the

robot discretizes space when predicting the future location of these objects, then the discretization makes the robot immediately become uncertain about the precise position of objects: each object could be anywhere within the discrete cell that it was observed to occupy.

In many cases, it is more practical to use a simple but uncertain rule rather than a complex but certain one, even if the true rule is deterministic and our modeling system has the fidelity to accommodate a complex rule. For example, the simple rule "Most birds fly" is cheap to develop and is broadly useful, while a rule of the form, "Birds fly, except for very young birds that have not yet learned to fly, sick or injured birds that have lost the ability to fly, flightless species of birds including the cassowary, ostrich and kiwi. . . " is expensive to develop, maintain and communicate, and after all of this effort is still very brittle and prone to failure.

Given that we need a means of representing and reasoning about uncertainty, it is not immediately obvious that probability theory can provide all of the tools we want for artificial intelligence applications. Probability theory was originally developed to analyze the frequencies of events. It is easy to see how probability theory can be used to study events like drawing a certain hand of cards in a game of poker. These kinds of events are often repeatable. When we say that an outcome has a probability p of occurring, it means that if we repeated the experiment (e.g., draw a hand of cards) infinitely many times, then proportion p of the repetitions would result in that outcome. This kind of reasoning does not seem immediately applicable to propositions that are not repeatable. If a doctor analyzes a patient and says that the patient has a 40% chance of having the flu, this means something very different—we can not make infinitely many replicas of the patient, nor is there any reason to believe that different replicas of the patient would present with the same symptoms yet have varying underlying conditions. In the case of the doctor diagnosing the patient, we use probability to represent a *degree of belief*, with 1 indicating absolute certainty that the patient has the flu and 0 indicating absolute certainty that the patient does not have the flu. The former kind of probability, related directly to the rates at which events occur, is known as *frequentist probability*, while the latter, related to qualitative levels of certainty, is known as *Bayesian probability*.

If we list several properties that we expect common sense reasoning about uncertainty to have, then the only way to satisfy those properties is to treat Bayesian probabilities as behaving exactly the same as frequentist probabilities. For example, if we want to compute the probability that a player will win a poker game given that she has a certain set of cards, we use exactly the same formulas as when we compute the probability that a patient has a disease given that she

has certain symptoms. For more details about why a small set of common sense assumptions implies that the same axioms must control both kinds of probability, see Ramsey (1926).

Probability can be seen as the extension of logic to deal with uncertainty. Logic provides a set of formal rules for determining what propositions are implied to be true or false given the assumption that some other set of propositions is true or false. Probability theory provides a set of formal rules for determining the likelihood of a proposition being true given the likelihood of other propositions.

3.2 Random Variables

A *random variable* is a variable that can take on different values randomly. We typically denote the random variable itself with a lower case letter in plain typeface, and the values it can take on with lower case script letters. For example, x_1 and x_2 are both possible values that the random variable x can take on. For vector-valued variables, we would write the random variable as $\mathbf{x}$ and one of its values as $\boldsymbol{x}$. On its own, a random variable is just a description of the states that are possible; it must be coupled with a probability distribution that specifies how likely each of these states are.

Random variables may be discrete or continuous. A discrete random variable is one that has a finite or countably infinite number of states. Note that these states are not necessarily the integers; they can also just be named states that are not considered to have any numerical value. A continuous random variable is associated with a real value.

3.3 Probability Distributions

A *probability distribution* is a description of how likely a random variable or set of random variables is to take on each of its possible states. The way we describe probability distributions depends on whether the variables are discrete or continuous.

3.3.1 Discrete Variables and Probability Mass Functions

A probability distribution over discrete variables may be described using a *probability mass function* (PMF). We typically denote probability mass functions with a capital P. Often we associate each random variable with a different probability

mass function and the reader must infer which probability mass function to use based on the identity of the random variable, rather than the name of the function; $P(\mathrm{x})$ is usually not the same as $P(\mathrm{y})$.

The probability mass function maps from a state of a random variable to the probability of that random variable taking on that state. The probability that $\mathrm{x} = x$ is denoted as $P(x)$, with a probability of 1 indicating that $\mathrm{x} = x$ is certain and a probability of 0 indicating that $\mathrm{x} = x$ is impossible. Sometimes to disambiguate which PMF to use, we write the name of the random variable explicitly: $P(\mathrm{x} = x)$. Sometimes we define a variable first, then use $\sim$ notation to specify which distribution it follows later: $\mathrm{x} \sim P(\mathrm{x})$.

Probability mass functions can act on many variables at the same time. Such a probability distribution over many variables is known as a *joint probability distribution*. $P(\mathrm{x} = x, \mathrm{y} = y)$ denotes the probability that $\mathrm{x} = x$ and $\mathrm{y} = y$ simultaneously. We may also write $P(x, y)$ for brevity.

To be a probability mass function on a random variable x, a function P must satisfy the following properties:

- The domain of P must be the set of all possible states of x.
- $\forall x \in \mathrm{x}, 0 \leq P(x) \leq 1$. An impossible event has probability 0 and no state can be less probable than that. Likewise, an event that is guaranteed to happen has probability 1, and no state can have a greater chance of occurring.
- $\sum_{x \in \mathrm{x}} P(x) = 1$. We refer to this property as being *normalized*. Without this property, we could obtain probabilities greater than one by computing the probability of one of many events occurring.

For example, consider a single discrete random variable x with k different states. We can place a *uniform distribution* on x—that is, make each of its states equally likely—by setting its probability mass function to

$$P(\mathrm{x} = x_i) = \frac{1}{k} \tag{3.1}$$

for all i. We can see that this fits the requirements for a probability mass function. The value $\frac{1}{k}$ is positive because k is a positive integer. We also see that

$$\sum_i P(\mathrm{x} = x_i) = \sum_i \frac{1}{k} = \frac{k}{k} = 1, \tag{3.2}$$

so the distribution is properly normalized.

3.3.2 Continuous Variables and Probability Density Functions

When working with continuous random variables, we describe probability distributions using a *probability density function (PDF)* rather than a probability mass function. To be a probability density function, a function p must satisfy the following properties:

- The domain of p must be the set of all possible states of x.
- $\forall x \in \mathrm{x}, p(x) \geq 0$. Note that we do not require $p(x) \leq 1$.
- $\int p(x)dx = 1$.

A probability density function $p(x)$ does not give the probability of a specific state directly, instead the probability of landing inside an infinitesimal region with volume δx is given by $p(x)\delta x$.

We can integrate the density function to find the actual probability mass of a set of points. Specifically, the probability that x lies in some set $\mathbb{S}$ is given by the integral of $p(x)$ over that set. In the univariate example, the probability that x lies in the interval $[a, b]$ is given by $\int_{[a,b]} p(x)dx$.

For an example of a probability density function corresponding to a specific probability density over a continuous random variable, consider a uniform distribution on an interval of the real numbers. We can do this with a function $u(x; a, b)$, where a and b are the endpoints of the interval, with $b > a$. The ";" notation means "parametrized by"; we consider x to be the argument of the function, while a and b are parameters that define the function. To ensure that there is no probability mass outside the interval, we say $u(x; a, b) = 0$ for all $x \notin [a, b]$. Within $[a, b]$, $u(x; a, b) = \frac{1}{b-a}$. We can see that this is nonnegative everywhere. Additionally, it integrates to 1. We often denote that x follows the uniform distribution on $[a, b]$ by writing $\mathrm{x} \sim U(a, b)$.

3.4 Marginal Probability

Sometimes we know the probability distribution over a set of variables and we want to know the probability distribution over just a subset of them. The probability distribution over the subset is known as the *marginal probability* distribution.

For example, suppose we have discrete random variables x and y, and we know $P(\mathrm{x}, \mathrm{y})$. We can find $P(\mathrm{x})$ with the *sum rule*:

$$\forall x \in \mathrm{x}, P(\mathrm{x} = x) = \sum_{y} P(\mathrm{x} = x, \mathrm{y} = y). \tag{3.3}$$

The name "marginal probability" comes from the process of computing marginal probabilities on paper. When the values of $P(\mathrm{x}, \mathrm{y})$ are written in a grid with different values of x in rows and different values of y in columns, it is natural to sum across a row of the grid, then write $P(x)$ in the margin of the paper just to the right of the row.

For continuous variables, we need to use integration instead of summation:

$$p(x) = \int p(x, y)dy. \tag{3.4}$$

3.5 Conditional Probability

In many cases, we are interested in the probability of some event, given that some other event has happened. This is called a *conditional probability*. We denote the conditional probability that $\mathrm{y} = y$ given $\mathrm{x} = x$ as $P(\mathrm{y} = y \mid \mathrm{x} = x)$. This conditional probability can be computed with the formula

$$P(\mathrm{y} = y \mid \mathrm{x} = x) = \frac{P(\mathrm{y} = y, \mathrm{x} = x)}{P(\mathrm{x} = x)}. \tag{3.5}$$

The conditional probability is only defined when $P(\mathrm{x} = x) > 0$. We cannot compute the conditional probability conditioned on an event that never happens.

It is important not to confuse conditional probability with computing what would happen if some action were undertaken. The conditional probability that a person is from Germany given that they speak German is quite high, but if a randomly selected person is taught to speak German, their country of origin does not change. Computing the consequences of an action is called making an *intervention query*. Intervention queries are the domain of *causal modeling*, which we do not explore in this book.

3.6 The Chain Rule of Conditional Probabilities

Any joint probability distribution over many random variables may be decomposed into conditional distributions over only one variable:

$$P(\mathrm{x}^{(1)}, \ldots, \mathrm{x}^{(n)}) = P(\mathrm{x}^{(1)}) \Pi_{i=2}^{n} P(\mathrm{x}^{(i)} \mid \mathrm{x}^{(1)}, \ldots, \mathrm{x}^{(i-1)}). \tag{3.6}$$

This observation is known as the *chain rule* or *product rule* of probability. It follows immediately from the definition of conditional probability in Eq. 3.5. For

example, applying the definition twice, we get

$$\begin{aligned} P(\mathrm{a}, \mathrm{b}, \mathrm{c}) &= P(\mathrm{a} \mid \mathrm{b}, \mathrm{c}) P(\mathrm{b}, \mathrm{c}) \\ P(\mathrm{b}, \mathrm{c}) &= P(\mathrm{b} \mid \mathrm{c}) P(\mathrm{c}) \\ P(\mathrm{a}, \mathrm{b}, \mathrm{c}) &= P(\mathrm{a} \mid \mathrm{b}, \mathrm{c}) P(\mathrm{b} \mid \mathrm{c}) P(\mathrm{c}). \end{aligned}$$

3.7 Independence and Conditional Independence

Two random variables x and y are *independent* if their probability distribution can be expressed as a product of two factors, one involving only x and one involving only y:

$$\forall x \in \mathrm{x}, y \in \mathrm{y},\ p(\mathrm{x} = x, \mathrm{y} = y) = p(\mathrm{x} = x) p(\mathrm{y} = y). \tag{3.7}$$

Two random variables x and y are *conditionally independent* given a random variable z if the conditional probability distribution over x and y factorizes in this way for every value of z:

$$\forall x \in \mathrm{x}, y \in \mathrm{y}, z \in \mathrm{z},\ p(\mathrm{x} = x, \mathrm{y} = y \mid \mathrm{z} = z) = p(\mathrm{x} = x \mid \mathrm{z} = z) p(\mathrm{y} = y \mid \mathrm{z} = z). \tag{3.8}$$

We can denote independence and conditional independence with compact notation: $\mathrm{x} \perp \mathrm{y}$ means that x and y are independent, while $\mathrm{x} \perp \mathrm{y} \mid \mathrm{z}$ means that x and y are conditionally independent given z.

3.8 Expectation, Variance and Covariance

The *expectation* or *expected value* of some function $f(x)$ with respect to a probability distribution $P(\mathrm{x})$ is the average or mean value that f takes on when x is drawn from P. For discrete variables this can be computed with a summation:

$$\mathbb{E}_{\mathrm{x} \sim P}[f(x)] = \sum_x P(x) f(x), \tag{3.9}$$

while for continuous variables, it is computed with an integral:

$$\mathbb{E}_{\mathrm{x} \sim p}[f(x)] = \int p(x) f(x) dx. \tag{3.10}$$

When the identity of the distribution is clear from the context, we may simply write the name of the random variable that the expectation is over, as in $\mathbb{E}_{\mathrm{x}}[f(x)]$. If it is clear which random variable the expectation is over, we may omit the subscript entirely, as in $\mathbb{E}[f(x)]$. By default, we can assume that $\mathbb{E}[\cdot]$ averages over the values of all the random variables inside the brackets. Likewise, when there is no ambiguity, we may omit the square brackets.

Expectations are linear, for example,

$$\mathbb{E}_{\mathrm{x}}[\alpha f(x) + \beta g(x)] = \alpha \mathbb{E}_{\mathrm{x}}[f(x)] + \beta \mathbb{E}_{\mathrm{x}}[g(x)], \tag{3.11}$$

when α and β are not dependent on x.

The *variance* gives a measure of how much the values of a function of a random variable x vary as we sample different values of x from its probability distribution:

$$\mathrm{Var}(f(x)) = \mathbb{E}\left[(f(x) - \mathbb{E}[f(x)])^2 \right]. \tag{3.12}$$

When the variance is low, the values of $f(x)$ cluster near their expected value. The square root of the variance is known as the *standard deviation*.

The *covariance* gives some sense of how much two values are linearly related to each other, as well as the scale of these variables:

$$\mathrm{Cov}(f(x), g(y)) = \mathbb{E}\left[(f(x) - \mathbb{E}\left[f(x)\right]) \left(g(y) - \mathbb{E}\left[g(y)\right]\right) \right]. \tag{3.13}$$

High absolute values of the covariance mean that the values change very much and are both far from their respective means at the same time. If the sign of the covariance is positive, then both variables tend to take on relatively high values simultaneously. If the sign of the covariance is negative, then one variable tends to take on a relatively high value at the times that the other takes on a relatively low value and vice versa. Other measures such as *correlation* normalize the contribution of each variable in order to measure only how much the variables are related, rather than also being affected by the scale of the separate variables.

The notions of covariance and dependence are related, but are in fact distinct concepts. They are related because two variables that are independent have zero covariance, and two variables that have non-zero covariance are dependent. However, independence is a distinct property from covariance. For two variables to have zero covariance, there must be no linear dependence between them. Independence is a stronger requirement than zero covariance, because independence also excludes nonlinear relationships. It is possible for two variables to be dependent but have zero covariance. For example, suppose we first sample a real number x from a uniform distribution over the interval $[-1, 1]$. We next sample a random variable

s. With probability $\frac{1}{2}$, we choose the value of s to be 1. Otherwise, we choose the value of s to be -1. We can then generate a random variable y by assigning $y = sx$. Clearly, x and y are not independent, because x completely determines the magnitude of y. However, $\text{Cov}(x, y) = 0$.

The *covariance matrix* of a random vector $\boldsymbol{x} \in \mathbb{R}^n$ is an $n \times n$ matrix, such that

$$\text{Cov}(\mathbf{x})_{i,j} = \text{Cov}(\mathrm{x}_i, \mathrm{x}_j). \tag{3.14}$$

The diagonal elements of the covariance give the variance:

$$\text{Cov}(\mathrm{x}_i, \mathrm{x}_i) = \text{Var}(\mathrm{x}_i). \tag{3.15}$$

3.9 Common Probability Distributions

Several simple probability distributions are useful in many contexts in machine learning.

3.9.1 Bernoulli Distribution

The *Bernoulli* distribution is a distribution over a single binary random variable. It is controlled by a single parameter $\phi \in [0, 1]$, which gives the probability of the random variable being equal to 1. It has the following properties:

$$P(\mathrm{x} = 1) = \phi \tag{3.16}$$

$$P(\mathrm{x} = 0) = 1 - \phi \tag{3.17}$$

$$P(\mathrm{x} = x) = \phi^x (1 - \phi)^{1-x} \tag{3.18}$$

$$\mathbb{E}_{\mathrm{x}}[\mathrm{x}] = \phi \tag{3.19}$$

$$\text{Var}_{\mathrm{x}}(\mathrm{x}) = \phi(1 - \phi) \tag{3.20}$$

3.9.2 Multinoulli Distribution

The *multinoulli* or *categorical* distribution is a distribution over a single discrete variable with k different states, where k is finite.[1] The multinoulli distribution is

[1] "Multinoulli" is a term that was recently coined by Gustavo Lacerdo and popularized by Murphy (2012). The multinoulli distribution is a special case of the *multinomial* distribution. A multinomial distribution is the distribution over vectors in $\{0, \ldots, n\}^k$ representing how many times each of the k categories is visited when n samples are drawn from a multinoulli distribution. Many texts use the term "multinomial" to refer to multinoulli distributions without clarifying that they refer only to the $n = 1$ case.

parametrized by a vector $\boldsymbol{p} \in [0, 1]^{k-1}$, where p_i gives the probability of the i-th state. The final, k-th state's probability is given by $1 - \mathbf{1}^\top \boldsymbol{p}$. Note that we must constrain $\mathbf{1}^\top \boldsymbol{p} \leq 1$. Multinoulli distributions are often used to refer to distributions over categories of objects, so we do not usually assume that state 1 has numerical value 1, etc. For this reason, we do not usually need to compute the expectation or variance of multinoulli-distributed random variables.

The Bernoulli and multinoulli distributions are sufficient to describe any distribution over their domain. This is because they model discrete variables for which it is feasible to simply enumerate all of the states. When dealing with continuous variables, there are uncountably many states, so any distribution described by a small number of parameters must impose strict limits on the distribution.

3.9.3 Gaussian Distribution

The most commonly used distribution over real numbers is the *normal distribution*, also known as the *Gaussian distribution*:

$$\mathcal{N}(x; \mu, \sigma^2) = \sqrt{\frac{1}{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right). \tag{3.21}$$

See Fig. 3.1 for a plot of the density function.

The two parameters $\mu \in \mathbb{R}$ and $\sigma \in (0, \infty)$ control the normal distribution. The parameter μ gives the coordinate of the central peak. This is also the mean of the distribution: $\mathbb{E}[\mathrm{x}] = \mu$. The standard deviation of the distribution is given by σ, and the variance by σ^2.

When we evaluate the PDF, we need to square and invert σ. When we need to frequently evaluate the PDF with different parameter values, a more efficient way of parametrizing the distribution is to use a parameter $\beta \in (0, \infty)$ to control the *precision* or inverse variance of the distribution:

$$\mathcal{N}(x; \mu, \beta^{-1}) = \sqrt{\frac{\beta}{2\pi}} \exp\left(-\frac{1}{2}\beta(x - \mu)^2\right). \tag{3.22}$$

Normal distributions are a sensible choice for many applications. In the absence of prior knowledge about what form a distribution over the real numbers should take, the normal distribution is a good default choice for two major reasons.

First, many distributions we wish to model are truly close to being normal distributions. The *central limit theorem* shows that the sum of many independent random variables is approximately normally distributed. This means that in

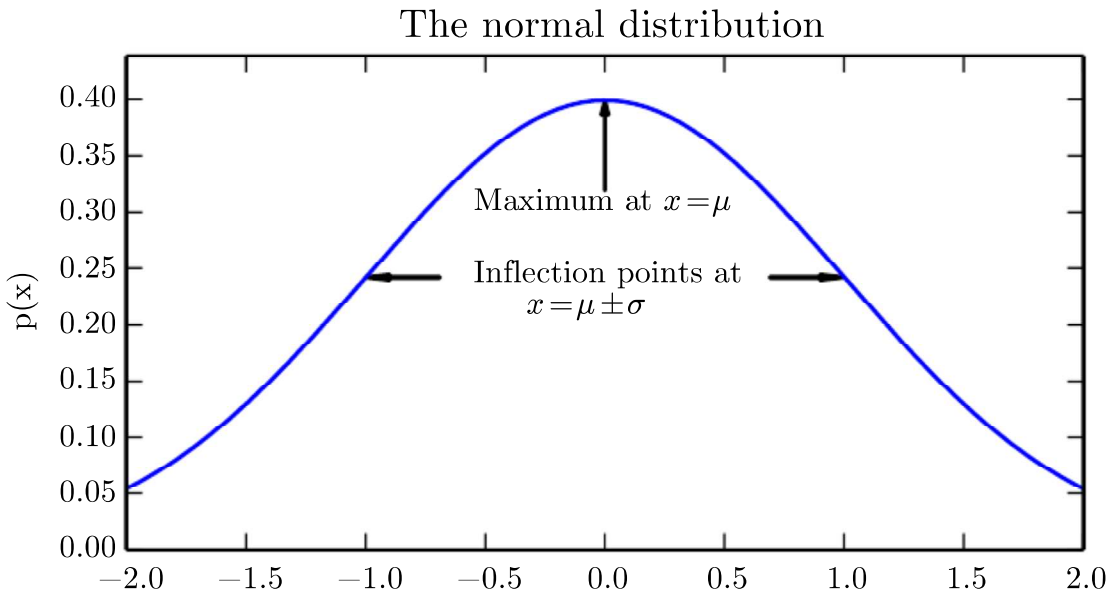


Figure 3.1: *The normal distribution*: The normal distribution $\mathcal{N}(x; \mu, \sigma^2)$ exhibits a classic "bell curve" shape, with the x coordinate of its central peak given by μ, and the width of its peak controlled by σ. In this example, we depict the *standard normal distribution*, with $\mu = 0$ and $\sigma = 1$.

practice, many complicated systems can be modeled successfully as normally distributed noise, even if the system can be decomposed into parts with more structured behavior.

Second, out of all possible probability distributions with the same variance, the normal distribution encodes the maximum amount of uncertainty over the real numbers. We can thus think of the normal distribution as being the one that inserts the least amount of prior knowledge into a model. Fully developing and justifying this idea requires more mathematical tools, and is postponed to Sec. 19.4.2.

The normal distribution generalizes to $\mathbb{R}^n$, in which case it is known as the *multivariate normal distribution*. It may be parametrized with a positive definite symmetric matrix $\boldsymbol{\Sigma}$:

$$\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sqrt{\frac{1}{(2\pi)^n \det(\boldsymbol{\Sigma})}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x} - \boldsymbol{\mu})\right). \tag{3.23}$$

The parameter $\boldsymbol{\mu}$ still gives the mean of the distribution, though now it is vector-valued. The parameter $\boldsymbol{\Sigma}$ gives the covariance matrix of the distribution. As in the univariate case, when we wish to evaluate the PDF several times for

many different values of the parameters, the covariance is not a computationally efficient way to parametrize the distribution, since we need to invert $\boldsymbol{\Sigma}$ to evaluate the PDF. We can instead use a *precision matrix* $\boldsymbol{\beta}$:

$$\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}, \boldsymbol{\beta}^{-1}) = \sqrt{\frac{\det(\boldsymbol{\beta})}{(2\pi)^n}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\top \boldsymbol{\beta}(\boldsymbol{x}-\boldsymbol{\mu})\right). \tag{3.24}$$

We often fix the covariance matrix to be a diagonal matrix. An even simpler version is the *isotropic* Gaussian distribution, whose covariance matrix is a scalar times the identity matrix.

3.9.4 Exponential and Laplace Distributions

In the context of deep learning, we often want to have a probability distribution with a sharp point at $x = 0$. To accomplish this, we can use the *exponential distribution*:

$$p(x; \lambda) = \lambda \mathbf{1}_{x \geq 0} \exp(-\lambda x). \tag{3.25}$$

The exponential distribution uses the indicator function $\mathbf{1}_{x \geq 0}$ to assign probability zero to all negative values of x.

A closely related probability distribution that allows us to place a sharp peak of probability mass at an arbitrary point μ is the *Laplace distribution*

$$\text{Laplace}(x; \mu, \gamma) = \frac{1}{2\gamma} \exp\left(-\frac{|x-\mu|}{\gamma}\right). \tag{3.26}$$

3.9.5 The Dirac Distribution and Empirical Distribution

In some cases, we wish to specify that all of the mass in a probability distribution clusters around a single point. This can be accomplished by defining a PDF using the Dirac delta function, $\delta(x)$:

$$p(x) = \delta(x - \mu). \tag{3.27}$$

The Dirac delta function is defined such that it is zero-valued everywhere except 0, yet integrates to 1. The Dirac delta function is not an ordinary function that associates each value x with a real-valued output, instead it is a different kind of mathematical object called a *generalized function* that is defined in terms of its properties when integrated. We can think of the Dirac delta function as being the limit point of a series of functions that put less and less mass on all points other than μ.

By defining $p(x)$ to be δ shifted by $-\mu$ we obtain an infinitely narrow and infinitely high peak of probability mass where $x = \mu$.

A common use of the Dirac delta distribution is as a component of an *empirical distribution*,

$$\hat{p}(\boldsymbol{x}) = \frac{1}{m} \sum_{i=1}^{m} \delta(\boldsymbol{x} - \boldsymbol{x}^{(i)}) \tag{3.28}$$

which puts probability mass $\frac{1}{m}$ on each of the m points $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}$ forming a given data set or collection of samples. The Dirac delta distribution is only necessary to define the empirical distribution over continuous variables. For discrete variables, the situation is simpler: an empirical distribution can be conceptualized as a multinoulli distribution, with a probability associated to each possible input value that is simply equal to the *empirical frequency* of that value in the training set.

We can view the empirical distribution formed from a dataset of training examples as specifying the distribution that we sample from when we train a model on this dataset. Another important perspective on the empirical distribution is that it is the probability density that maximizes the likelihood of the training data (see Sec. 5.5).

3.9.6 Mixtures of Distributions

It is also common to define probability distributions by combining other simpler probability distributions. One common way of combining distributions is to construct a *mixture distribution*. A mixture distribution is made up of several component distributions. On each trial, the choice of which component distribution generates the sample is determined by sampling a component identity from a multinoulli distribution:

$$P(\mathrm{x}) = \sum_{i} P(\mathrm{c} = i) P(\mathrm{x} \mid \mathrm{c} = i) \tag{3.29}$$

where $P(\mathrm{c})$ is the multinoulli distribution over component identities.

We have already seen one example of a mixture distribution: the empirical distribution over real-valued variables is a mixture distribution with one Dirac component for each training example.

The mixture model is one simple strategy for combining probability distributions to create a richer distribution. In Chapter 16, we explore the art of building complex probability distributions from simple ones in more detail.

The mixture model allows us to briefly glimpse a concept that will be of paramount importance later—the *latent variable*. A latent variable is a random variable that we cannot observe directly. The component identity variable c of the mixture model provides an example. Latent variables may be related to x through the joint distribution, in this case, $P(\mathrm{x}, \mathrm{c}) = P(\mathrm{x} \mid \mathrm{c})P(\mathrm{c})$. The distribution $P(\mathrm{c})$ over the latent variable and the distribution $P(\mathrm{x} \mid \mathrm{c})$ relating the latent variables to the visible variables determines the shape of the distribution $P(\mathrm{x})$ even though it is possible to describe $P(\mathrm{x})$ without reference to the latent variable. Latent variables are discussed further in Sec. 16.5.

A very powerful and common type of mixture model is the *Gaussian mixture* model, in which the components $p(\mathbf{x} \mid \mathrm{c} = i)$ are Gaussians. Each component has a separately parametrized mean $\boldsymbol{\mu}^{(i)}$ and covariance $\boldsymbol{\Sigma}^{(i)}$. Some mixtures can have more constraints. For example, the covariances could be shared across components via the constraint $\boldsymbol{\Sigma}^{(i)} = \boldsymbol{\Sigma} \forall i$. As with a single Gaussian distribution, the mixture of Gaussians might constrain the covariance matrix for each component to be diagonal or isotropic.

In addition to the means and covariances, the parameters of a Gaussian mixture specify the *prior probability* $\alpha_i = P(\mathrm{c} = i)$ given to each component i. The word "prior" indicates that it expresses the model's beliefs about c **before** it has observed $\mathbf{x}$. By comparison, $P(\mathrm{c} \mid \boldsymbol{x})$ is a *posterior probability*, because it is computed **after** observation of $\mathbf{x}$. A Gaussian mixture model is a *universal approximator* of densities, in the sense that any smooth density can be approximated with any specific, non-zero amount of error by a Gaussian mixture model with enough components.

Fig. 3.2 shows samples from a Gaussian mixture model.

3.10 Useful Properties of Common Functions

Certain functions arise often while working with probability distributions, especially the probability distributions used in deep learning models.

One of these functions is the *logistic sigmoid*:

$$\sigma(x) = \frac{1}{1 + \exp(-x)}. \tag{3.30}$$

The logistic sigmoid is commonly used to produce the ϕ parameter of a Bernoulli distribution because its range is $(0,1)$, which lies within the valid range of values for the ϕ parameter. See Fig. 3.3 for a graph of the sigmoid function. The sigmoid

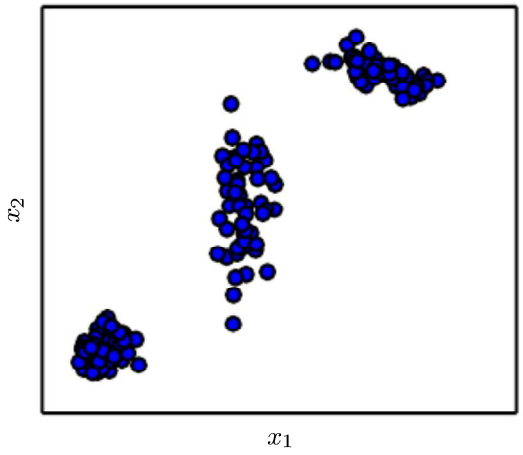


Figure 3.2: Samples from a Gaussian mixture model. In this example, there are three components. From left to right, the first component has an isotropic covariance matrix, meaning it has the same amount of variance in each direction. The second has a diagonal covariance matrix, meaning it can control the variance separately along each axis-aligned direction. This example has more variance along the x_2 axis than along the x_1 axis. The third component has a full-rank covariance matrix, allowing it to control the variance separately along an arbitrary basis of directions.

function *saturates* when its argument is very positive or very negative, meaning that the function becomes very flat and insensitive to small changes in its input.

Another commonly encountered function is the *softplus* function (Dugas *et al.*, 2001):

$$\zeta(x) = \log\left(1 + \exp(x)\right). \tag{3.31}$$

The softplus function can be useful for producing the β or σ parameter of a normal distribution because its range is $(0, \infty)$. It also arises commonly when manipulating expressions involving sigmoids. The name of the softplus function comes from the fact that it is a smoothed or "softened" version of

$$x^+ = \max(0, x). \tag{3.32}$$

See Fig. 3.4 for a graph of the softplus function.

The following properties are all useful enough that you may wish to memorize them:

$$\sigma(x) = \frac{\exp(x)}{\exp(x) + \exp(0)} \tag{3.33}$$

$$\frac{d}{dx}\sigma(x) = \sigma(x)(1 - \sigma(x)) \tag{3.34}$$

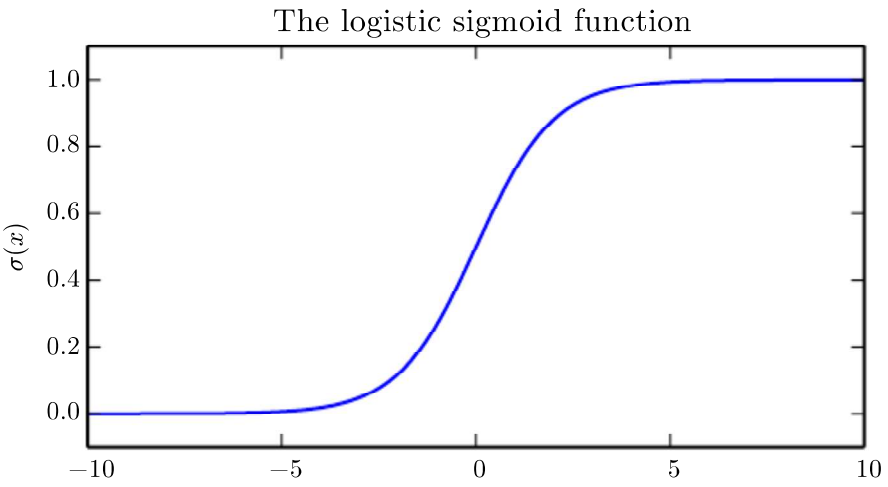


Figure 3.3: The logistic sigmoid function.

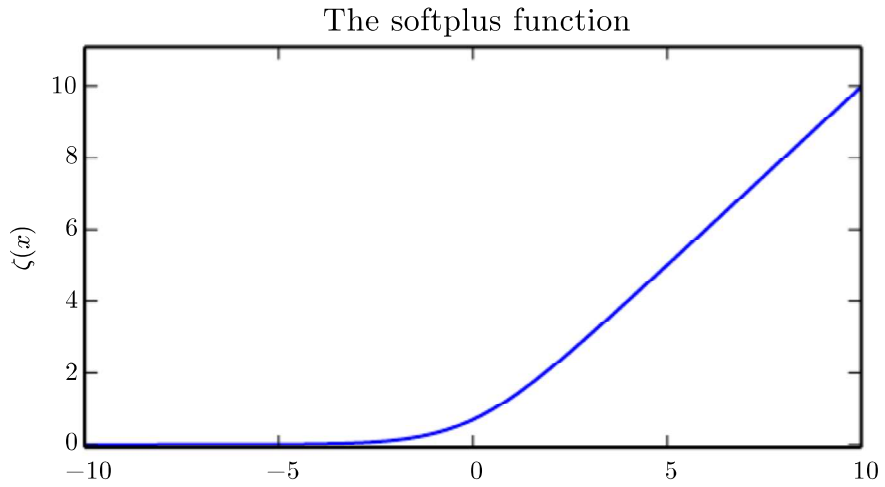


Figure 3.4: The softplus function.

$$1 - \sigma(x) = \sigma(-x) \tag{3.35}$$

$$\log \sigma(x) = -\zeta(-x) \tag{3.36}$$

$$\frac{d}{dx}\zeta(x) = \sigma(x) \tag{3.37}$$

$$\forall x \in (0, 1),\ \sigma^{-1}(x) = \log\left(\frac{x}{1-x}\right) \tag{3.38}$$

$$\forall x > 0,\ \zeta^{-1}(x) = \log\left(\exp(x) - 1\right) \tag{3.39}$$

$$\zeta(x) = \int_{-\infty}^{x} \sigma(y)dy \tag{3.40}$$

$$\zeta(x) - \zeta(-x) = x \tag{3.41}$$

The function $\sigma^{-1}(x)$ is called the *logit* in statistics, but this term is more rarely used in machine learning.

Eq. 3.41 provides extra justification for the name "softplus." The softplus function is intended as a smoothed version of the *positive part* function, $x^+ = \max\{0, x\}$. The positive part function is the counterpart of the *negative part* function, $x^- = \max\{0, -x\}$. To obtain a smooth function that is analogous to the negative part, one can use $\zeta(-x)$. Just as x can be recovered from its positive part and negative part via the identity $x^+ - x^- = x$, it is also possible to recover x using the same relationship between $\zeta(x)$ and $\zeta(-x)$, as shown in Eq. 3.41.

3.11 Bayes' Rule

We often find ourselves in a situation where we know $P(\mathrm{y} \mid \mathrm{x})$ and need to know $P(\mathrm{x} \mid \mathrm{y})$. Fortunately, if we also know $P(\mathrm{x})$, we can compute the desired quantity using *Bayes' rule*:

$$P(\mathrm{x} \mid \mathrm{y}) = \frac{P(\mathrm{x})P(\mathrm{y} \mid \mathrm{x})}{P(\mathrm{y})}. \tag{3.42}$$

Note that while $P(\mathrm{y})$ appears in the formula, it is usually feasible to compute $P(\mathrm{y}) = \sum_x P(\mathrm{y} \mid x)P(x)$, so we do not need to begin with knowledge of $P(\mathrm{y})$.

Bayes' rule is straightforward to derive from the definition of conditional probability, but it is useful to know the name of this formula since many texts refer to it by name. It is named after the Reverend Thomas Bayes, who first discovered a special case of the formula. The general version presented here was independently discovered by Pierre-Simon Laplace.

3.12 Technical Details of Continuous Variables

A proper formal understanding of continuous random variables and probability density functions requires developing probability theory in terms of a branch of mathematics known as *measure theory*. Measure theory is beyond the scope of this textbook, but we can briefly sketch some of the issues that measure theory is employed to resolve.

In Sec. 3.3.2, we saw that the probability of a continuous vector-valued $\mathbf{x}$ lying in some set $\mathbb{S}$ is given by the integral of $p(\boldsymbol{x})$ over the set $\mathbb{S}$. Some choices of set $\mathbb{S}$ can produce paradoxes. For example, it is possible to construct two sets $\mathbb{S}_1$ and $\mathbb{S}_2$ such that $p(\boldsymbol{x} \in \mathbb{S}_1) + p(\boldsymbol{x} \in \mathbb{S}_2) > 1$ but $\mathbb{S}_1 \cap \mathbb{S}_2 = \emptyset$. These sets are generally constructed making very heavy use of the infinite precision of real numbers, for example by making fractal-shaped sets or sets that are defined by transforming the set of rational numbers.[2] One of the key contributions of measure theory is to provide a characterization of the set of sets that we can compute the probability of without encountering paradoxes. In this book, we only integrate over sets with relatively simple descriptions, so this aspect of measure theory never becomes a relevant concern.

For our purposes, measure theory is more useful for describing theorems that apply to most points in $\mathbb{R}^n$ but do not apply to some corner cases. Measure theory provides a rigorous way of describing that a set of points is negligibly small. Such a set is said to have "*measure zero*." We do not formally define this concept in this textbook. However, it is useful to understand the intuition that a set of measure zero occupies no volume in the space we are measuring. For example, within $\mathbb{R}^2$, a line has measure zero, while a filled polygon has positive measure. Likewise, an individual point has measure zero. Any union of countably many sets that each have measure zero also has measure zero (so the set of all the rational numbers has measure zero, for instance).

Another useful term from measure theory is "*almost everywhere*." A property that holds almost everywhere holds throughout all of space except for on a set of measure zero. Because the exceptions occupy a negligible amount of space, they can be safely ignored for many applications. Some important results in probability theory hold for all discrete values but only hold "almost everywhere" for continuous values.

Another technical detail of continuous variables relates to handling continuous random variables that are deterministic functions of one another. Suppose we have two random variables, $\mathbf{x}$ and $\mathbf{y}$, such that $\boldsymbol{y} = g(\boldsymbol{x})$, where g is an invertible, con-

[2]The Banach-Tarski theorem provides a fun example of such sets.

tinuous, differentiable transformation. One might expect that $p_y(\boldsymbol{y}) = p_x(g^{-1}(\boldsymbol{y}))$. This is actually not the case.

As a simple example, suppose we have scalar random variables x and y. Suppose $y = \frac{x}{2}$ and $x \sim U(0, 1)$. If we use the rule $p_y(y) = p_x(2y)$ then p_y will be 0 everywhere except the interval $[0, \frac{1}{2}]$, and it will be 1 on this interval. This means

$$\int p_y(y)dy = \frac{1}{2}, \tag{3.43}$$

which violates the definition of a probability distribution.

This common mistake is wrong because it fails to account for the distortion of space introduced by the function g. Recall that the probability of $\boldsymbol{x}$ lying in an infinitesimally small region with volume $\delta\boldsymbol{x}$ is given by $p(\boldsymbol{x})\delta\boldsymbol{x}$. Since g can expand or contract space, the infinitesimal volume surrounding $\boldsymbol{x}$ in $\boldsymbol{x}$ space may have different volume in $\boldsymbol{y}$ space.

To see how to correct the problem, we return to the scalar case. We need to preserve the property

$$|p_y(g(x))dy| = |p_x(x)dx|. \tag{3.44}$$

Solving from this, we obtain

$$p_y(y) = p_x(g^{-1}(y)) \left|\frac{\partial x}{\partial y}\right| \tag{3.45}$$

or equivalently

$$p_x(x) = p_y(g(x)) \left|\frac{\partial g(x)}{\partial x}\right|. \tag{3.46}$$

In higher dimensions, the derivative generalizes to the determinant of the *Jacobian matrix*—the matrix with $J_{i,j} = \frac{\partial x_i}{\partial y_j}$. Thus, for real-valued vectors $\boldsymbol{x}$ and $\boldsymbol{y}$,

$$p_x(\boldsymbol{x}) = p_y(g(\boldsymbol{x})) \left|\det\left(\frac{\partial g(\boldsymbol{x})}{\partial \boldsymbol{x}}\right)\right|. \tag{3.47}$$

3.13 Information Theory

Information theory is a branch of applied mathematics that revolves around quantifying how much information is present in a signal. It was originally invented to study sending messages from discrete alphabets over a noisy channel, such as communication via radio transmission. In this context, information theory tells how to design optimal codes and calculate the expected length of messages sampled from

specific probability distributions using various encoding schemes. In the context of machine learning, we can also apply information theory to continuous variables where some of these message length interpretations do not apply. This field is fundamental to many areas of electrical engineering and computer science. In this textbook, we mostly use a few key ideas from information theory to characterize probability distributions or quantify similarity between probability distributions. For more detail on information theory, see Cover and Thomas (2006) or MacKay (2003).

The basic intuition behind information theory is that learning that an unlikely event has occurred is more informative than learning that a likely event has occurred. A message saying "the sun rose this morning" is so uninformative as to be unnecessary to send, but a message saying "there was a solar eclipse this morning" is very informative.

We would like to quantify information in a way that formalizes this intuition. Specifically,

- Likely events should have low information content, and in the extreme case, events that are guaranteed to happen should have no information content whatsoever.
- Less likely events should have higher information content.
- Independent events should have additive information. For example, finding out that a tossed coin has come up as heads twice should convey twice as much information as finding out that a tossed coin has come up as heads once.

In order to satisfy all three of these properties, we define the *self-information* of an event $\mathrm{x} = x$ to be

$$I(x) = -\log P(x). \tag{3.48}$$

In this book, we always use log to mean the natural logarithm, with base e. Our definition of $I(x)$ is therefore written in units of *nats*. One nat is the amount of information gained by observing an event of probability $\frac{1}{e}$. Other texts use base-2 logarithms and units called *bits* or *shannons*; information measured in bits is just a rescaling of information measured in nats.

When x is continuous, we use the same definition of information by analogy, but some of the properties from the discrete case are lost. For example, an event with unit density still has zero information, despite not being an event that is guaranteed to occur.

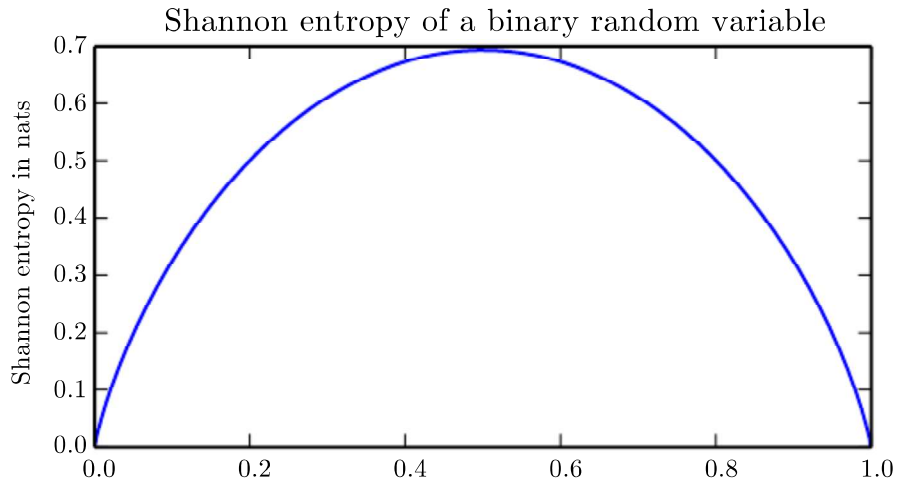


Figure 3.5: This plot shows how distributions that are closer to deterministic have low Shannon entropy while distributions that are close to uniform have high Shannon entropy. On the horizontal axis, we plot p, the probability of a binary random variable being equal to 1. The entropy is given by $(p-1)\log(1-p) - p\log p$. When p is near 0, the distribution is nearly deterministic, because the random variable is nearly always 0. When$p$ is near 1, the distribution is nearly deterministic, because the random variable is nearly always 1. When $p = 0.5$, the entropy is maximal, because the distribution is uniform over the two outcomes.

Self-information deals only with a single outcome. We can quantify the amount of uncertainty in an entire probability distribution using the *Shannon entropy*:

$$H(\mathrm{x}) = \mathbb{E}_{\mathrm{x}\sim P}[I(x)] = -\mathbb{E}_{\mathrm{x}\sim P}[\log P(x)]. \tag{3.49}$$

also denoted $H(P)$. In other words, the Shannon entropy of a distribution is the expected amount of information in an event drawn from that distribution. It gives a lower bound on the number of bits (if the logarithm is base 2, otherwise the units are different) needed on average to encode symbols drawn from a distribution P. Distributions that are nearly deterministic (where the outcome is nearly certain) have low entropy; distributions that are closer to uniform have high entropy. See Fig. 3.5 for a demonstration. When x is continuous, the Shannon entropy is known as the *differential entropy*.

If we have two separate probability distributions $P(\mathrm{x})$ and $Q(\mathrm{x})$ over the same random variable x, we can measure how different these two distributions are using the *Kullback-Leibler (KL) divergence*:

$$D_{\mathrm{KL}}(P\|Q) = \mathbb{E}_{\mathrm{x}\sim P}\left[\log \frac{P(x)}{Q(x)}\right] = \mathbb{E}_{\mathrm{x}\sim P}\left[\log P(x) - \log Q(x)\right]. \tag{3.50}$$

In the case of discrete variables, it is the extra amount of information (measured in bits if we use the base 2 logarithm, but in machine learning we usually use nats and the natural logarithm) needed to send a message containing symbols drawn from probability distribution P, when we use a code that was designed to minimize the length of messages drawn from probability distribution Q.

The KL divergence has many useful properties, most notably that it is non-negative. The KL divergence is 0 if and only if P and Q are the same distribution in the case of discrete variables, or equal "almost everywhere" in the case of continuous variables. Because the KL divergence is non-negative and measures the difference between two distributions, it is often conceptualized as measuring some sort of distance between these distributions. However, it is not a true distance measure because it is not symmetric: $D_{\mathrm{KL}}(P\|Q) \neq D_{\mathrm{KL}}(Q\|P)$ for some P and Q. This asymmetry means that there are important consequences to the choice of whether to use $D_{\mathrm{KL}}(P\|Q)$ or $D_{\mathrm{KL}}(Q\|P)$. See Fig. 3.6 for more detail.

A quantity that is closely related to the KL divergence is the *cross-entropy* $H(P,Q) = H(P) + D_{\mathrm{KL}}(P\|Q)$, which is similar to the KL divergence but lacking the term on the left:

$$H(P,Q) = -\mathbb{E}_{\mathrm{x}\sim P} \log Q(x). \tag{3.51}$$

Minimizing the cross-entropy with respect to Q is equivalent to minimizing the KL divergence, because Q does not participate in the omitted term.

When computing many of these quantities, it is common to encounter expressions of the form $0 \log 0$. By convention, in the context of information theory, we treat these expressions as $\lim_{x\to 0} x \log x = 0$.

3.14 Structured Probabilistic Models

Machine learning algorithms often involve probability distributions over a very large number of random variables. Often, these probability distributions involve direct interactions between relatively few variables. Using a single function to describe the entire joint probability distribution can be very inefficient (both computationally and statistically).

Instead of using a single function to represent a probability distribution, we can split a probability distribution into many factors that we multiply together. For example, suppose we have three random variables: a, b and c. Suppose that a influences the value of b and b influences the value of c, but that a and c are independent given b. We can represent the probability distribution over all three

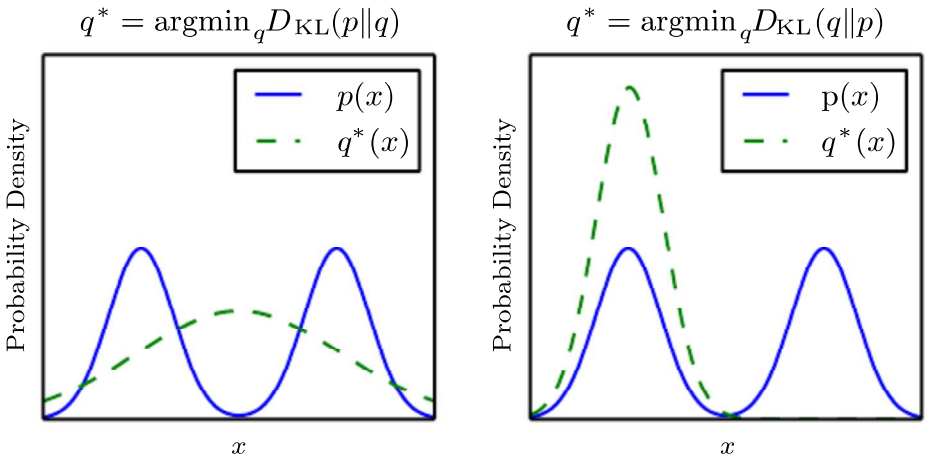


Figure 3.6: The KL divergence is asymmetric. Suppose we have a distribution $p(x)$ and wish to approximate it with another distribution $q(x)$. We have the choice of minimizing either $D_{\text{KL}}(p\|q)$ or $D_{\text{KL}}(q\|p)$. We illustrate the effect of this choice using a mixture of two Gaussians for p, and a single Gaussian for q. The choice of which direction of the KL divergence to use is problem-dependent. Some applications require an approximation that usually places high probability anywhere that the true distribution places high probability, while other applications require an approximation that rarely places high probability anywhere that the true distribution places low probability. The choice of the direction of the KL divergence reflects which of these considerations takes priority for each application. *(Left)* The effect of minimizing $D_{\text{KL}}(p\|q)$. In this case, we select a q that has high probability where p has high probability. When p has multiple modes, q chooses to blur the modes together, in order to put high probability mass on all of them. *(Right)* The effect of minimizing $D_{\text{KL}}(q\|p)$. In this case, we select a q that has low probability where p has low probability. When p has multiple modes that are sufficiently widely separated, as in this figure, the KL divergence is minimized by choosing a single mode, in order to avoid putting probability mass in the low-probability areas between modes of p. Here, we illustrate the outcome when q is chosen to emphasize the left mode. We could also have achieved an equal value of the KL divergence by choosing the right mode. If the modes are not separated by a sufficiently strong low probability region, then this direction of the KL divergence can still choose to blur the modes.

variables as a product of probability distributions over two variables:

$$p(\mathrm{a}, \mathrm{b}, \mathrm{c}) = p(\mathrm{a})p(\mathrm{b} \mid \mathrm{a})p(\mathrm{c} \mid \mathrm{b}). \tag{3.52}$$

These factorizations can greatly reduce the number of parameters needed to describe the distribution. Each factor uses a number of parameters that is exponential in the number of variables in the factor. This means that we can greatly reduce the cost of representing a distribution if we are able to find a factorization into distributions over fewer variables.

We can describe these kinds of factorizations using graphs. Here we use the word "graph" in the sense of graph theory: a set of vertices that may be connected to each other with edges. When we represent the factorization of a probability distribution with a graph, we call it a *structured probabilistic model* or *graphical model*.

There are two main kinds of structured probabilistic models: directed and undirected. Both kinds of graphical models use a graph $\mathcal{G}$ in which each node in the graph corresponds to a random variable, and an edge connecting two random variables means that the probability distribution is able to represent direct interactions between those two random variables.

Directed models use graphs with directed edges, and they represent factorizations into conditional probability distributions, as in the example above. Specifically, a directed model contains one factor for every random variable x_i in the distribution, and that factor consists of the conditional distribution over x_i given the parents of x_i, denoted $Pa_{\mathcal{G}}(\mathrm{x}_i)$:

$$p(\mathbf{x}) = \prod_i p\left(\mathrm{x}_i \mid Pa_{\mathcal{G}}\left(\mathrm{x}_i\right)\right). \tag{3.53}$$

See Fig. 3.7 for an example of a directed graph and the factorization of probability distributions it represents.

Undirected models use graphs with undirected edges, and they represent factorizations into a set of functions; unlike in the directed case, these functions are usually not probability distributions of any kind. Any set of nodes that are all connected to each other in $\mathcal{G}$ is called a clique. Each clique $\mathcal{C}^{(i)}$ in an undirected model is associated with a factor $\phi^{(i)}(\mathcal{C}^{(i)})$. These factors are just functions, not probability distributions. The output of each factor must be non-negative, but there is no constraint that the factor must sum or integrate to 1 like a probability distribution.

The probability of a configuration of random variables is *proportional* to the product of all of these factors—assignments that result in larger factor values are

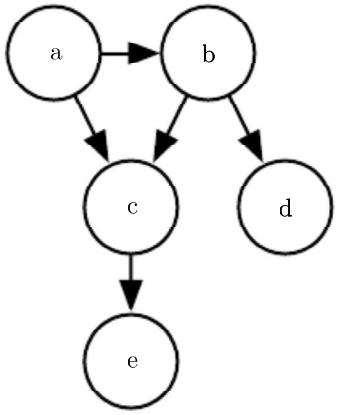


Figure 3.7: A directed graphical model over random variables a, b, c, d and e. This graph corresponds to probability distributions that can be factored as

$$p(\mathrm{a}, \mathrm{b}, \mathrm{c}, \mathrm{d}, \mathrm{e}) = p(\mathrm{a})p(\mathrm{b} \mid \mathrm{a})p(\mathrm{c} \mid \mathrm{a}, \mathrm{b})p(\mathrm{d} \mid \mathrm{b})p(\mathrm{e} \mid \mathrm{c}). \tag{3.54}$$

This graph allows us to quickly see some properties of the distribution. For example, a and c interact directly, but a and e interact only indirectly via c.

more likely. Of course, there is no guarantee that this product will sum to 1. We therefore divide by a normalizing constant Z, defined to be the sum or integral over all states of the product of the ϕ functions, in order to obtain a normalized probability distribution:

$$p(\mathbf{x}) = \frac{1}{Z} \prod_i \phi^{(i)}\left(\mathcal{C}^{(i)}\right). \tag{3.55}$$

See Fig. 3.8 for an example of an undirected graph and the factorization of probability distributions it represents.

Keep in mind that these graphical representations of factorizations are a language for describing probability distributions. They are not mutually exclusive families of probability distributions. Being directed or undirected is not a property of a probability distribution; it is a property of a particular *description* of a probability distribution, but any probability distribution may be described in both ways.

Throughout Part I and Part II of this book, we will use structured probabilistic models merely as a language to describe which direct probabilistic relationships different machine learning algorithms choose to represent. No further understanding of structured probabilistic models is needed until the discussion of research topics, in Part III, where we will explore structured probabilistic models in much greater detail.

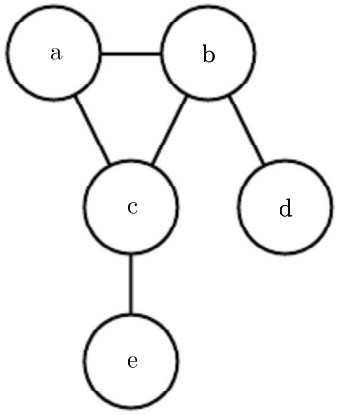


Figure 3.8: An undirected graphical model over random variables a, b, c, d and e. This graph corresponds to probability distributions that can be factored as

$$p(\mathrm{a}, \mathrm{b}, \mathrm{c}, \mathrm{d}, \mathrm{e}) = \frac{1}{Z}\phi^{(1)}(\mathrm{a}, \mathrm{b}, \mathrm{c})\phi^{(2)}(\mathrm{b}, \mathrm{d})\phi^{(3)}(\mathrm{c}, \mathrm{e}). \tag{3.56}$$

This graph allows us to quickly see some properties of the distribution. For example, a and c interact directly, but a and e interact only indirectly via c.

This chapter has reviewed the basic concepts of probability theory that are most relevant to deep learning. One more set of fundamental mathematical tools remains: numerical methods.

Chapter 4

Numerical Computation

Machine learning algorithms usually require a high amount of numerical computation. This typically refers to algorithms that solve mathematical problems by methods that update estimates of the solution via an iterative process, rather than analytically deriving a formula providing a symbolic expression for the correct solution. Common operations include optimization (finding the value of an argument that minimizes or maximizes a function) and solving systems of linear equations. Even just evaluating a mathematical function on a digital computer can be difficult when the function involves real numbers, which cannot be represented precisely using a finite amount of memory.

4.1 Overflow and Underflow

The fundamental difficulty in performing continuous math on a digital computer is that we need to represent infinitely many real numbers with a finite number of bit patterns. This means that for almost all real numbers, we incur some approximation error when we represent the number in the computer. In many cases, this is just rounding error. Rounding error is problematic, especially when it compounds across many operations, and can cause algorithms that work in theory to fail in practice if they are not designed to minimize the accumulation of rounding error.

One form of rounding error that is particularly devastating is *underflow*. Underflow occurs when numbers near zero are rounded to zero. Many functions behave qualitatively differently when their argument is zero rather than a small positive number. For example, we usually want to avoid division by zero (some software

environments will raise exceptions when this occurs, others will return a result with a placeholder not-a-number value) or taking the logarithm of zero (this is usually treated as $-\infty$, which then becomes not-a-number if it is used for many further arithmetic operations).

Another highly damaging form of numerical error is *overflow*. Overflow occurs when numbers with large magnitude are approximated as ∞ or $-\infty$. Further arithmetic will usually change these infinite values into not-a-number values.

One example of a function that must be stabilized against underflow and overflow is the softmax function. The softmax function is often used to predict the probabilities associated with a multinoulli distribution. The softmax function is defined to be

$$\text{softmax}(\boldsymbol{x})_i = \frac{\exp(x_i)}{\sum_{j=1}^{n} \exp(x_j)}. \tag{4.1}$$

Consider what happens when all of the x_i are equal to some constant c. Analytically, we can see that all of the outputs should be equal to $\frac{1}{n}$. Numerically, this may not occur when c has large magnitude. If c is very negative, then $\exp(c)$ will underflow. This means the denominator of the softmax will become 0, so the final result is undefined. When c is very large and positive, $\exp(c)$ will overflow, again resulting in the expression as a whole being undefined. Both of these difficulties can be resolved by instead evaluating $\text{softmax}(\boldsymbol{z})$ where $\boldsymbol{z} = \boldsymbol{x} - \max_i x_i$. Simple algebra shows that the value of the softmax function is not changed analytically by adding or subtracting a scalar from the input vector. Subtracting $\max_i x_i$ results in the largest argument to exp being 0, which rules out the possibility of overflow. Likewise, at least one term in the denominator has a value of 1, which rules out the possibility of underflow in the denominator leading to a division by zero.

There is still one small problem. Underflow in the numerator can still cause the expression as a whole to evaluate to zero. This means that if we implement $\log \text{softmax}(\boldsymbol{x})$ by first running the softmax subroutine then passing the result to the log function, we could erroneously obtain $-\infty$. Instead, we must implement a separate function that calculates $\log \text{softmax}$ in a numerically stable way. The $\log \text{softmax}$ function can be stabilized using the same trick as we used to stabilize the softmax function.

For the most part, we do not explicitly detail all of the numerical considerations involved in implementing the various algorithms described in this book. Developers of low-level libraries should keep numerical issues in mind when implementing deep learning algorithms. Most readers of this book can simply rely on low-level libraries that provide stable implementations. In some cases, it is possible to implement a new algorithm and have the new implementation automatically

stabilized. Theano (Bergstra *et al.*, 2010; Bastien *et al.*, 2012) is an example of a software package that automatically detects and stabilizes many common numerically unstable expressions that arise in the context of deep learning.

4.2 Poor Conditioning

Conditioning refers to how rapidly a function changes with respect to small changes in its inputs. Functions that change rapidly when their inputs are perturbed slightly can be problematic for scientific computation because rounding errors in the inputs can result in large changes in the output.

Consider the function $f(\boldsymbol{x}) = \boldsymbol{A}^{-1}\boldsymbol{x}$. When $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ has an eigenvalue decomposition, its *condition number* is

$$\max_{i,j} \left| \frac{\lambda_i}{\lambda_j} \right|. \tag{4.2}$$

This is the ratio of the magnitude of the largest and smallest eigenvalue. When this number is large, matrix inversion is particularly sensitive to error in the input.

This sensitivity is an intrinsic property of the matrix itself, not the result of rounding error during matrix inversion. Poorly conditioned matrices amplify pre-existing errors when we multiply by the true matrix inverse. In practice, the error will be compounded further by numerical errors in the inversion process itself.

4.3 Gradient-Based Optimization

Most deep learning algorithms involve optimization of some sort. Optimization refers to the task of either minimizing or maximizing some function $f(\boldsymbol{x})$ by altering $\boldsymbol{x}$. We usually phrase most optimization problems in terms of minimizing $f(\boldsymbol{x})$. Maximization may be accomplished via a minimization algorithm by minimizing $-f(\boldsymbol{x})$.

The function we want to minimize or maximize is called the *objective function* or *criterion*. When we are minimizing it, we may also call it the *cost function*, *loss function*, or *error function*. In this book, we use these terms interchangeably, though some machine learning publications assign special meaning to some of these terms.

We often denote the value that minimizes or maximizes a function with a superscript $*$. For example, we might say $\boldsymbol{x}^* = \arg\min f(\boldsymbol{x})$.

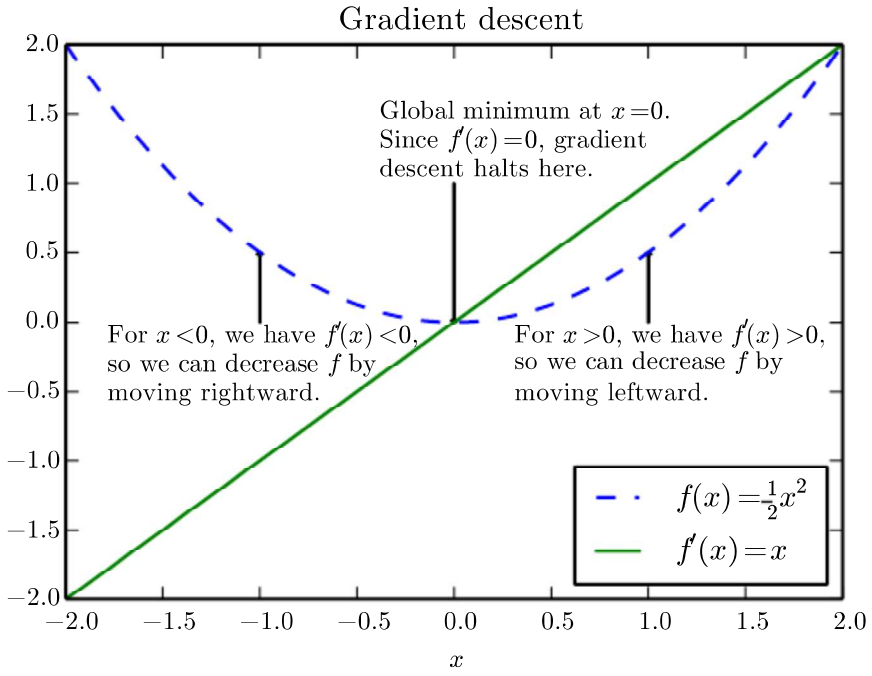


Figure 4.1: An illustration of how the derivatives of a function can be used to follow the function downhill to a minimum. This technique is called *gradient descent*.

We assume the reader is already familiar with calculus, but provide a brief review of how calculus concepts relate to optimization here.

Suppose we have a function $y = f(x)$, where both x and y are real numbers. The *derivative* of this function is denoted as $f'(x)$ or as $\frac{dy}{dx}$. The derivative $f'(x)$ gives the slope of $f(x)$ at the point x. In other words, it specifies how to scale a small change in the input in order to obtain the corresponding change in the output: $f(x + \epsilon) \approx f(x) + \epsilon f'(x)$.

The derivative is therefore useful for minimizing a function because it tells us how to change x in order to make a small improvement in y. For example, we know that $f(x - \epsilon \operatorname{sign}(f'(x)))$ is less than $f(x)$ for small enough ϵ. We can thus reduce $f(x)$ by moving x in small steps with opposite sign of the derivative. This technique is called *gradient descent* (Cauchy, 1847). See Fig. 4.1 for an example of this technique.

When $f'(x) = 0$, the derivative provides no information about which direction to move. Points where $f'(x) = 0$ are known as *critical points* or *stationary points*. A *local minimum* is a point where $f(x)$ is lower than at all neighboring points, so it is no longer possible to decrease $f(x)$ by making infinitesimal steps. A *local maximum* is a point where $f(x)$ is higher than at all neighboring points, so it is

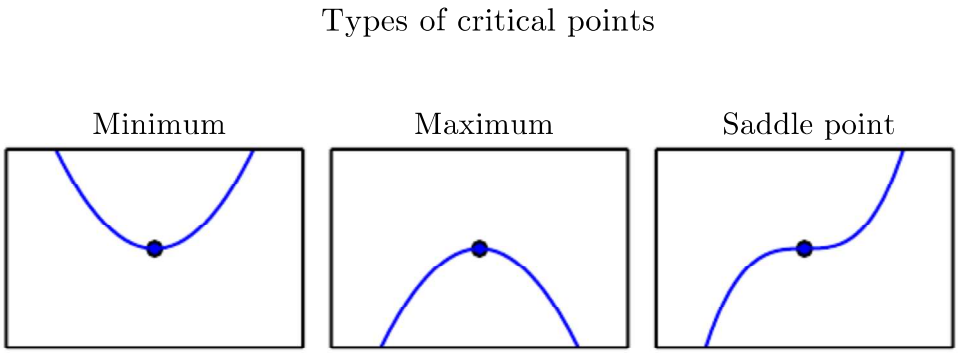


Figure 4.2: Examples of each of the three types of critical points in 1-D. A critical point is a point with zero slope. Such a point can either be a local minimum, which is lower than the neighboring points, a local maximum, which is higher than the neighboring points, or a saddle point, which has neighbors that are both higher and lower than the point itself.

not possible to increase $f(x)$ by making infinitesimal steps. Some critical points are neither maxima nor minima. These are known as *saddle points*. See Fig. 4.2 for examples of each type of critical point.

A point that obtains the absolute lowest value of $f(x)$ is a *global minimum*. It is possible for there to be only one global minimum or multiple global minima of the function. It is also possible for there to be local minima that are not globally optimal. In the context of deep learning, we optimize functions that may have many local minima that are not optimal, and many saddle points surrounded by very flat regions. All of this makes optimization very difficult, especially when the input to the function is multidimensional. We therefore usually settle for finding a value of f that is very low, but not necessarily minimal in any formal sense. See Fig. 4.3 for an example.

We often minimize functions that have multiple inputs: $f : \mathbb{R}^n \to \mathbb{R}$. For the concept of "minimization" to make sense, there must still be only one (scalar) output.

For functions with multiple inputs, we must make use of the concept of *partial derivatives*. The partial derivative $\frac{\partial}{\partial x_i} f(\boldsymbol{x})$ measures how f changes as only the variable x_i increases at point $\boldsymbol{x}$. The *gradient* generalizes the notion of derivative to the case where the derivative is with respect to a vector: the gradient of f is the vector containing all of the partial derivatives, denoted $\nabla_{\boldsymbol{x}} f(\boldsymbol{x})$. Element i of the gradient is the partial derivative of f with respect to x_i. In multiple dimensions,

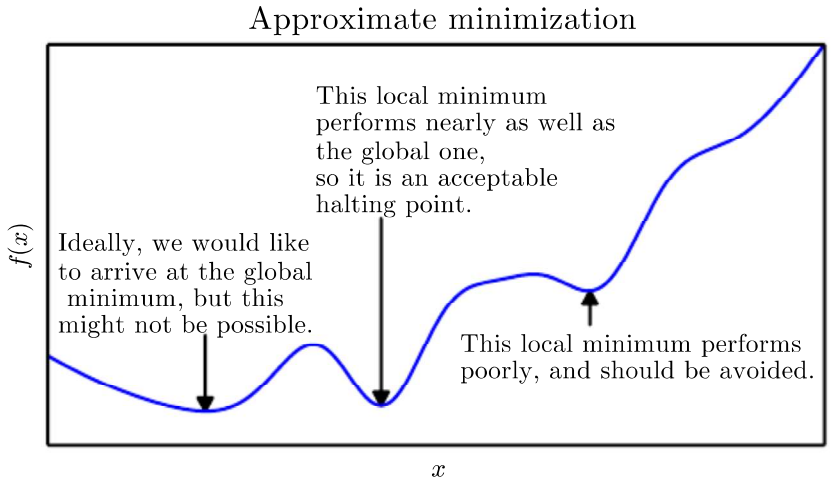


Figure 4.3: Optimization algorithms may fail to find a global minimum when there are multiple local minima or plateaus present. In the context of deep learning, we generally accept such solutions even though they are not truly minimal, so long as they correspond to significantly low values of the cost function.

critical points are points where every element of the gradient is equal to zero.

The *directional derivative* in direction $\boldsymbol{u}$ (a unit vector) is the slope of the function f in direction u. In other words, the directional derivative is the derivative of the function $f(\boldsymbol{x} + \alpha \boldsymbol{u})$ with respect to α, evaluated at $\alpha = 0$. Using the chain rule, we can see that $\frac{\partial}{\partial \alpha} f(\boldsymbol{x} + \alpha \boldsymbol{u}) = \boldsymbol{u}^\top \nabla_{\boldsymbol{x}} f(\boldsymbol{x})$.

To minimize f, we would like to find the direction in which f decreases the fastest. We can do this using the directional derivative:

$$\min_{\boldsymbol{u}, \boldsymbol{u}^\top \boldsymbol{u} = 1} \boldsymbol{u}^\top \nabla_{\boldsymbol{x}} f(\boldsymbol{x}) \tag{4.3}$$

$$= \min_{\boldsymbol{u}, \boldsymbol{u}^\top \boldsymbol{u} = 1} ||\boldsymbol{u}||_2 ||\nabla_{\boldsymbol{x}} f(\boldsymbol{x})||_2 \cos \theta \tag{4.4}$$

where θ is the angle between $\boldsymbol{u}$ and the gradient. Substituting in $||\boldsymbol{u}||_2 = 1$ and ignoring factors that do not depend on $\boldsymbol{u}$, this simplifies to $\min_{\boldsymbol{u}} \cos \theta$. This is minimized when $\boldsymbol{u}$ points in the opposite direction as the gradient. In other words, the gradient points directly uphill, and the negative gradient points directly downhill. We can decrease f by moving in the direction of the negative gradient. This is known as the *method of steepest descent* or *gradient descent*.

Steepest descent proposes a new point

$$\boldsymbol{x}' = \boldsymbol{x} - \epsilon \nabla_{\boldsymbol{x}} f(\boldsymbol{x}) \tag{4.5}$$

where ϵ is the *learning rate*, a positive scalar determining the size of the step. We can choose ϵ in several different ways. A popular approach is to set ϵ to a small constant. Sometimes, we can solve for the step size that makes the directional derivative vanish. Another approach is to evaluate $f\left(\boldsymbol{x} - \epsilon \nabla_{\boldsymbol{x}} f(\boldsymbol{x})\right)$ for several values of ϵ and choose the one that results in the smallest objective function value. This last strategy is called a *line search*.

Steepest descent converges when every element of the gradient is zero (or, in practice, very close to zero). In some cases, we may be able to avoid running this iterative algorithm, and just jump directly to the critical point by solving the equation $\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) = 0$ for $\boldsymbol{x}$.

Although gradient descent is limited to optimization in continuous spaces, the general concept of making small moves (that are approximately the best small move) towards better configurations can be generalized to discrete spaces. Ascending an objective function of discrete parameters is called *hill climbing* (Russel and Norvig, 2003).

4.3.1 Beyond the Gradient: Jacobian and Hessian Matrices

Sometimes we need to find all of the partial derivatives of a function whose input and output are both vectors. The matrix containing all such partial derivatives is known as a *Jacobian matrix*. Specifically, if we have a function $\boldsymbol{f} : \mathbb{R}^m \rightarrow \mathbb{R}^n$, then the Jacobian matrix $\boldsymbol{J} \in \mathbb{R}^{n \times m}$ of $\boldsymbol{f}$ is defined such that $J_{i,j} = \frac{\partial}{\partial x_j} f(\boldsymbol{x})_i$.

We are also sometimes interested in a derivative of a derivative. This is known as a *second derivative*. For example, for a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, the derivative with respect to x_i of the derivative of f with respect to x_j is denoted as $\frac{\partial^2}{\partial x_i \partial x_j} f$. In a single dimension, we can denote $\frac{d^2}{dx^2} f$ by $f''(x)$. The second derivative tells us how the first derivative will change as we vary the input. This is important because it tells us whether a gradient step will cause as much of an improvement as we would expect based on the gradient alone. We can think of the second derivative as measuring *curvature*. Suppose we have a quadratic function (many functions that arise in practice are not quadratic but can be approximated well as quadratic, at least locally). If such a function has a second derivative of zero, then there is no curvature. It is a perfectly flat line, and its value can be predicted using only the gradient. If the gradient is 1, then we can make a step of size ϵ along the negative gradient, and the cost function will decrease by ϵ. If the second derivative is negative, the function curves downward, so the cost function will actually decrease by more than ϵ. Finally, if the second derivative is positive, the function curves upward, so the cost function can decrease by less than ϵ. See Fig.

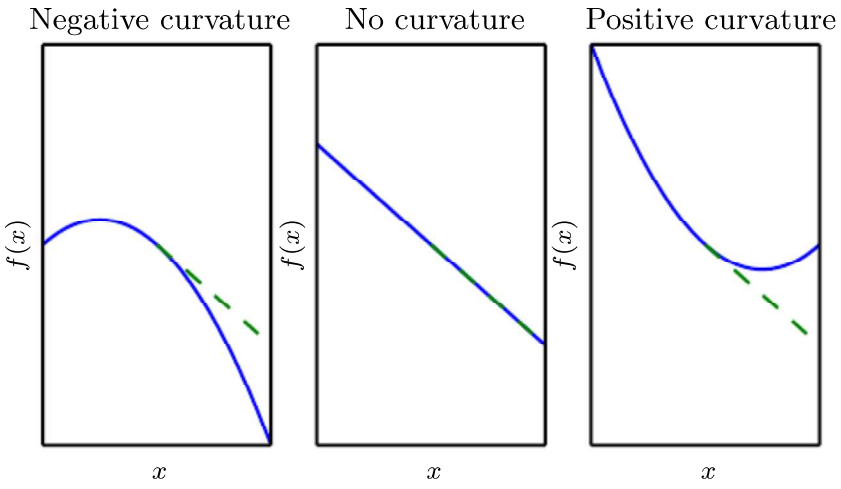


Figure 4.4: The second derivative determines the curvature of a function. Here we show quadratic functions with various curvature. The dashed line indicates the value of the cost function we would expect based on the gradient information alone as we make a gradient step downhill. In the case of negative curvature, the cost function actually decreases faster than the gradient predicts. In the case of no curvature, the gradient predicts the decrease correctly. In the case of positive curvature, the function decreases slower than expected and eventually begins to increase, so too large of step sizes can actually increase the function inadvertently.

4.4 to see how different forms of curvature affect the relationship between the value of the cost function predicted by the gradient and the true value.

When our function has multiple input dimensions, there are many second derivatives. These derivatives can be collected together into a matrix called the *Hessian matrix*. The Hessian matrix $\boldsymbol{H}(f)(\boldsymbol{x})$ is defined such that

$$\boldsymbol{H}(f)(\boldsymbol{x})_{i,j} = \frac{\partial^2}{\partial x_i \partial x_j} f(\boldsymbol{x}). \tag{4.6}$$

Equivalently, the Hessian is the Jacobian of the gradient.

Anywhere that the second partial derivatives are continuous, the differential operators are commutative, i.e. their order can be swapped:

$$\frac{\partial^2}{\partial x_i \partial x_j} f(\boldsymbol{x}) = \frac{\partial^2}{\partial x_j \partial x_i} f(\boldsymbol{x}). \tag{4.7}$$

This implies that $H_{i,j} = H_{j,i}$, so the Hessian matrix is symmetric at such points. Most of the functions we encounter in the context of deep learning have a symmetric Hessian almost everywhere. Because the Hessian matrix is real and symmetric, we can decompose it into a set of real eigenvalues and an orthogonal basis of

eigenvectors. The second derivative in a specific direction represented by a unit vector $\boldsymbol{d}$ is given by $\boldsymbol{d}^\top \boldsymbol{H} \boldsymbol{d}$. When $\boldsymbol{d}$ is an eigenvector of $\boldsymbol{H}$, the second derivative in that direction is given by the corresponding eigenvalue. For other directions of $\boldsymbol{d}$, the directional second derivative is a weighted average of all of the eigenvalues, with weights between 0 and 1, and eigenvectors that have smaller angle with $\boldsymbol{d}$ receiving more weight. The maximum eigenvalue determines the maximum second derivative and the minimum eigenvalue determines the minimum second derivative.

The (directional) second derivative tells us how well we can expect a gradient descent step to perform. We can make a second-order Taylor series approximation to the function $f(\boldsymbol{x})$ around the current point $\boldsymbol{x}^{(0)}$:

$$f(\boldsymbol{x}) \approx f(\boldsymbol{x}^{(0)}) + (\boldsymbol{x} - \boldsymbol{x}^{(0)})^\top \boldsymbol{g} + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}^{(0)})^\top \boldsymbol{H}(\boldsymbol{x} - \boldsymbol{x}^{(0)}). \tag{4.8}$$

where $\boldsymbol{g}$ is the gradient and $\boldsymbol{H}$ is the Hessian at $\boldsymbol{x}^{(0)}$. If we use a learning rate of ϵ, then the new point $\boldsymbol{x}$ will be given by $\boldsymbol{x}^{(0)} - \epsilon \boldsymbol{g}$. Substituting this into our approximation, we obtain

$$f(\boldsymbol{x}^{(0)} - \epsilon \boldsymbol{g}) \approx f(\boldsymbol{x}^{(0)}) - \epsilon \boldsymbol{g}^\top \boldsymbol{g} + \frac{1}{2}\epsilon^2 \boldsymbol{g}^\top \boldsymbol{H} \boldsymbol{g}. \tag{4.9}$$

There are three terms here: the original value of the function, the expected improvement due to the slope of the function, and the correction we must apply to account for the curvature of the function. When this last term is too large, the gradient descent step can actually move uphill. When $\boldsymbol{g}^\top \boldsymbol{H} \boldsymbol{g}$ is zero or negative, the Taylor series approximation predicts that increasing ϵ forever will decrease f forever. In practice, the Taylor series is unlikely to remain accurate for large ϵ, so one must resort to more heuristic choices of ϵ in this case. When $\boldsymbol{g}^\top \boldsymbol{H} \boldsymbol{g}$ is positive, solving for the optimal step size that decreases the Taylor series approximation of the function the most yields

$$\epsilon^* = \frac{\boldsymbol{g}^\top \boldsymbol{g}}{\boldsymbol{g}^\top \boldsymbol{H} \boldsymbol{g}}. \tag{4.10}$$

In the worst case, when $\boldsymbol{g}$ aligns with the eigenvector of $\boldsymbol{H}$ corresponding to the maximal eigenvalue $\lambda_{\max}$, then this optimal step size is given by $\frac{1}{\lambda_{\max}}$. To the extent that the function we minimize can be approximated well by a quadratic function, the eigenvalues of the Hessian thus determine the scale of the learning rate.

The second derivative can be used to determine whether a critical point is a local maximum, a local minimum, or saddle point. Recall that on a critical point, $f'(x) = 0$. When $f''(x) > 0$, this means that $f'(x)$ increases as we move to the right, and $f'(x)$ decreases as we move to the left. This means $f'(x - \epsilon) < 0$ and

$f'(x+\epsilon) > 0$ for small enough ϵ. In other words, as we move right, the slope begins to point uphill to the right, and as we move left, the slope begins to point uphill to the left. Thus, when $f'(x) = 0$ and $f''(x) > 0$, we can conclude that x is a local minimum. Similarly, when $f'(x) = 0$ and $f''(x) < 0$, we can conclude that x is a local maximum. This is known as the *second derivative test*. Unfortunately, when $f''(x) = 0$, the test is inconclusive. In this case x may be a saddle point, or a part of a flat region.

In multiple dimensions, we need to examine all of the second derivatives of the function. Using the eigendecomposition of the Hessian matrix, we can generalize the second derivative test to multiple dimensions. At a critical point, where $\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) = 0$, we can examine the eigenvalues of the Hessian to determine whether the critical point is a local maximum, local minimum, or saddle point. When the Hessian is positive definite (all its eigenvalues are positive), the point is a local minimum. This can be seen by observing that the directional second derivative in any direction must be positive, and making reference to the univariate second derivative test. Likewise, when the Hessian is negative definite (all its eigenvalues are negative), the point is a local maximum. In multiple dimensions, it is actually possible to find positive evidence of saddle points in some cases. When at least one eigenvalue is positive and at least one eigenvalue is negative, we know that $\boldsymbol{x}$ is a local maximum on one cross section of f but a local minimum on another cross section. See Fig. 4.5 for an example. Finally, the multidimensional second derivative test can be inconclusive, just like the univariate version. The test is inconclusive whenever all of the non-zero eigenvalues have the same sign, but at least one eigenvalue is zero. This is because the univariate second derivative test is inconclusive in the cross section corresponding to the zero eigenvalue.

In multiple dimensions, there can be a wide variety of different second derivatives at a single point, because there is a different second derivative for each direction. The condition number of the Hessian measures how much the second derivatives vary. When the Hessian has a poor condition number, gradient descent performs poorly. This is because in one direction, the derivative increases rapidly, while in another direction, it increases slowly. Gradient descent is unaware of this change in the derivative so it does not know that it needs to explore preferentially in the direction where the derivative remains negative for longer. It also makes it difficult to choose a good step size. The step size must be small enough to avoid overshooting the minimum and going uphill in directions with strong positive curvature. This usually means that the step size is too small to make significant progress in other directions with less curvature. See Fig. 4.6 for an example.

This issue can be resolved by using information from the Hessian matrix to

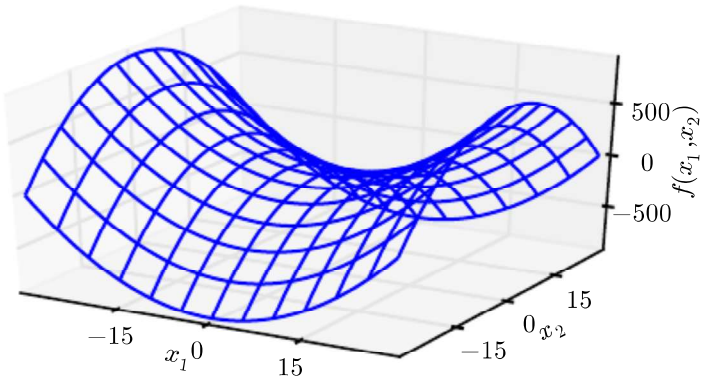


Figure 4.5: A saddle point containing both positive and negative curvature. The function in this example is $f(\boldsymbol{x}) = x_1^2 - x_2^2$. Along the axis corresponding to x_1, the function curves upward. This axis is an eigenvector of the Hessian and has a positive eigenvalue. Along the axis corresponding to x_2, the function curves downward. This direction is an eigenvector of the Hessian with negative eigenvalue. The name "saddle point" derives from the saddle-like shape of this function. This is the quintessential example of a function with a saddle point. In more than one dimension, it is not necessary to have an eigenvalue of 0 in order to get a saddle point: it is only necessary to have both positive and negative eigenvalues. We can think of a saddle point with both signs of eigenvalues as being a local maximum within one cross section and a local minimum within another cross section.

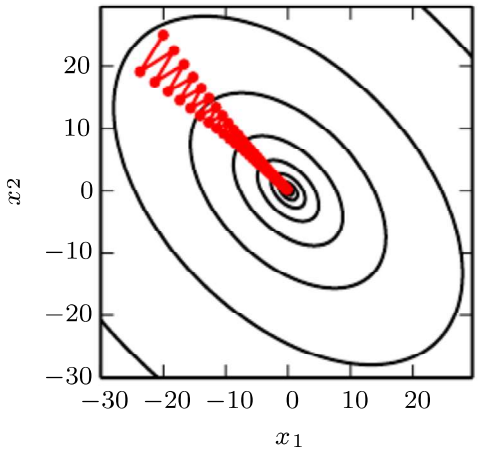


Figure 4.6: Gradient descent fails to exploit the curvature information contained in the Hessian matrix. Here we use gradient descent to minimize a quadratic function $f(\boldsymbol{x})$ whose Hessian matrix has condition number 5. This means that the direction of most curvature has five times more curvature than the direction of least curvature. In this case, the most curvature is in the direction $[1, 1]^\top$ and the least curvature is in the direction $[1, -1]^\top$. The red lines indicate the path followed by gradient descent. This very elongated quadratic function resembles a long canyon. Gradient descent wastes time repeatedly descending canyon walls, because they are the steepest feature. Because the step size is somewhat too large, it has a tendency to overshoot the bottom of the function and thus needs to descend the opposite canyon wall on the next iteration. The large positive eigenvalue of the Hessian corresponding to the eigenvector pointed in this direction indicates that this directional derivative is rapidly increasing, so an optimization algorithm based on the Hessian could predict that the steepest direction is not actually a promising search direction in this context.

guide the search. The simplest method for doing so is known as *Newton's method*. Newton's method is based on using a second-order Taylor series expansion to approximate $f(\boldsymbol{x})$ near some point $\boldsymbol{x}^{(0)}$:

$$f(\boldsymbol{x}) \approx f(\boldsymbol{x}^{(0)}) + (\boldsymbol{x} - \boldsymbol{x}^{(0)})^\top \nabla_{\boldsymbol{x}} f(\boldsymbol{x}^{(0)}) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}^{(0)})^\top \boldsymbol{H}(f)(\boldsymbol{x}^{(0)})(\boldsymbol{x} - \boldsymbol{x}^{(0)}). \quad (4.11)$$

If we then solve for the critical point of this function, we obtain:

$$\boldsymbol{x}^* = \boldsymbol{x}^{(0)} - \boldsymbol{H}(f)(\boldsymbol{x}^{(0)})^{-1} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}^{(0)}). \quad (4.12)$$

When f is a positive definite quadratic function, Newton's method consists of applying Eq. 4.12 once to jump to the minimum of the function directly. When f is not truly quadratic but can be locally approximated as a positive definite quadratic, Newton's method consists of applying Eq. 4.12 multiple times. Iteratively updating the approximation and jumping to the minimum of the approximation can reach the critical point much faster than gradient descent would. This is a useful property near a local minimum, but it can be a harmful property near a saddle point. As discussed in Sec. 8.2.3, Newton's method is only appropriate when the nearby critical point is a minimum (all the eigenvalues of the Hessian are positive), whereas gradient descent is not attracted to saddle points unless the gradient points toward them.

Optimization algorithms such as gradient descent that use only the gradient are called *first-order optimization algorithms*. Optimization algorithms such as Newton's method that also use the Hessian matrix are called *second-order optimization algorithms* (Nocedal and Wright, 2006).

The optimization algorithms employed in most contexts in this book are applicable to a wide variety of functions, but come with almost no guarantees. This is because the family of functions used in deep learning is quite complicated. In many other fields, the dominant approach to optimization is to design optimization algorithms for a limited family of functions.

In the context of deep learning, we sometimes gain some guarantees by restricting ourselves to functions that are either *Lipschitz continuous* or have Lipschitz continuous derivatives. A Lipschitz continuous function is a function f whose rate of change is bounded by a *Lipschitz constant* $\mathcal{L}$:

$$\forall \boldsymbol{x}, \forall \boldsymbol{y}, |f(\boldsymbol{x}) - f(\boldsymbol{y})| \leq \mathcal{L} ||\boldsymbol{x} - \boldsymbol{y}||_2. \quad (4.13)$$

This property is useful because it allows us to quantify our assumption that a small change in the input made by an algorithm such as gradient descent will have a small change in the output. Lipschitz continuity is also a fairly weak constraint,

and many optimization problems in deep learning can be made Lipschitz continuous with relatively minor modifications.

Perhaps the most successful field of specialized optimization is *convex optimization*. Convex optimization algorithms are able to provide many more guarantees by making stronger restrictions. Convex optimization algorithms are applicable only to convex functions—functions for which the Hessian is positive semidefinite everywhere. Such functions are well-behaved because they lack saddle points and all of their local minima are necessarily global minima. However, most problems in deep learning are difficult to express in terms of convex optimization. Convex optimization is used only as a subroutine of some deep learning algorithms. Ideas from the analysis of convex optimization algorithms can be useful for proving the convergence of deep learning algorithms. However, in general, the importance of convex optimization is greatly diminished in the context of deep learning. For more information about convex optimization, see Boyd and Vandenberghe (2004) or Rockafellar (1997).

4.4 Constrained Optimization

Sometimes we wish not only to maximize or minimize a function $f(\boldsymbol{x})$ over all possible values of $\boldsymbol{x}$. Instead we may wish to find the maximal or minimal value of $f(\boldsymbol{x})$ for values of $\boldsymbol{x}$ in some set $\mathbb{S}$. This is known as *constrained optimization*. Points $\boldsymbol{x}$ that lie within the set $\mathbb{S}$ are called *feasible* points in constrained optimization terminology.

We often wish to find a solution that is small in some sense. A common approach in such situations is to impose a norm constraint, such as $||\boldsymbol{x}|| \leq 1$.

One simple approach to constrained optimization is simply to modify gradient descent taking the constraint into account. If we use a small constant step size ϵ, we can make gradient descent steps, then project the result back into $\mathbb{S}$. If we use a line search, we can search only over step sizes ϵ that yield new $\boldsymbol{x}$ points that are feasible, or we can project each point on the line back into the constraint region. When possible, this method can be made more efficient by projecting the gradient into the tangent space of the feasible region before taking the step or beginning the line search (Rosen, 1960).

A more sophisticated approach is to design a different, unconstrained optimization problem whose solution can be converted into a solution to the original, constrained optimization problem. For example, if we want to minimize $f(\boldsymbol{x})$ for $\boldsymbol{x} \in \mathbb{R}^2$ with $\boldsymbol{x}$ constrained to have exactly unit L^2 norm, we can instead minimize

$g(\theta) = f([\cos\theta, \sin\theta]^\top)$ with respect to θ, then return $[\cos\theta, \sin\theta]$ as the solution to the original problem. This approach requires creativity; the transformation between optimization problems must be designed specifically for each case we encounter.

The *Karush–Kuhn–Tucker* (KKT) approach[1] provides a very general solution to constrained optimization. With the KKT approach, we introduce a new function called the *generalized Lagrangian* or *generalized Lagrange function*.

To define the Lagrangian, we first need to describe $\mathbb{S}$ in terms of equations and inequalities. We want a description of $\mathbb{S}$ in terms of m functions $g^{(i)}$ and n functions $h^{(j)}$ so that $\mathbb{S} = \{\boldsymbol{x} \mid \forall i, g^{(i)}(\boldsymbol{x}) = 0 \text{ and } \forall j, h^{(j)}(\boldsymbol{x}) \leq 0\}$. The equations involving $g^{(i)}$ are called the *equality constraints* and the inequalities involving $h^{(j)}$ are called *inequality constraints*.

We introduce new variables λ_i and α_j for each constraint, these are called the KKT multipliers. The generalized Lagrangian is then defined as

$$L(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\alpha}) = f(\boldsymbol{x}) + \sum_i \lambda_i g^{(i)}(\boldsymbol{x}) + \sum_j \alpha_j h^{(j)}(\boldsymbol{x}). \tag{4.14}$$

We can now solve a constrained minimization problem using unconstrained optimization of the generalized Lagrangian. Observe that, so long as at least one feasible point exists and $f(\boldsymbol{x})$ is not permitted to have value ∞, then

$$\min_{\boldsymbol{x}} \max_{\boldsymbol{\lambda}} \max_{\boldsymbol{\alpha}, \boldsymbol{\alpha} \geq 0} L(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\alpha}). \tag{4.15}$$

has the same optimal objective function value and set of optimal points $\boldsymbol{x}$ as

$$\min_{\boldsymbol{x} \in \mathbb{S}} f(\boldsymbol{x}). \tag{4.16}$$

This follows because any time the constraints are satisfied,

$$\max_{\boldsymbol{\lambda}} \max_{\boldsymbol{\alpha}, \boldsymbol{\alpha} \geq 0} L(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\alpha}) = f(\boldsymbol{x}), \tag{4.17}$$

while any time a constraint is violated,

$$\max_{\boldsymbol{\lambda}} \max_{\boldsymbol{\alpha}, \boldsymbol{\alpha} \geq 0} L(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\alpha}) = \infty. \tag{4.18}$$

These properties guarantee that no infeasible point will ever be optimal, and that the optimum within the feasible points is unchanged.

[1] The KKT approach generalizes the method of *Lagrange multipliers* which allows equality constraints but not inequality constraints.

To perform constrained maximization, we can construct the generalized Lagrange function of $-f(\boldsymbol{x})$, which leads to this optimization problem:

$$\min_{\boldsymbol{x}} \max_{\boldsymbol{\lambda}} \max_{\boldsymbol{\alpha}, \boldsymbol{\alpha} \geq 0} -f(\boldsymbol{x}) + \sum_i \lambda_i g^{(i)}(\boldsymbol{x}) + \sum_j \alpha_j h^{(j)}(\boldsymbol{x}). \tag{4.19}$$

We may also convert this to a problem with maximization in the outer loop:

$$\max_{\boldsymbol{x}} \min_{\boldsymbol{\lambda}} \min_{\boldsymbol{\alpha}, \boldsymbol{\alpha} \geq 0} f(\boldsymbol{x}) + \sum_i \lambda_i g^{(i)}(\boldsymbol{x}) - \sum_j \alpha_j h^{(j)}(\boldsymbol{x}). \tag{4.20}$$

The sign of the term for the equality constraints does not matter; we may define it with addition or subtraction as we wish, because the optimization is free to choose any sign for each λ_i.

The inequality constraints are particularly interesting. We say that a constraint $h^{(i)}(\boldsymbol{x})$ is *active* if $h^{(i)}(\boldsymbol{x}^*) = 0$. If a constraint is not active, then the solution to the problem found using that constraint would remain at least a local solution if that constraint were removed. It is possible that an inactive constraint excludes other solutions. For example, a convex problem with an entire region of globally optimal points (a wide, flat, region of equal cost) could have a subset of this region eliminated by constraints, or a non-convex problem could have better local stationary points excluded by a constraint that is inactive at convergence. However, the point found at convergence remains a stationary point whether or not the inactive constraints are included. Because an inactive $h^{(i)}$ has negative value, then the solution to $\min_{\boldsymbol{x}} \max_{\boldsymbol{\lambda}} \max_{\boldsymbol{\alpha}, \boldsymbol{\alpha} \geq 0} L(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\alpha})$ will have $\alpha_i = 0$. We can thus observe that at the solution, $\boldsymbol{\alpha} \boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}$. In other words, for all i, we know that at least one of the constraints $\alpha_i \geq 0$ and $h^{(i)}(\boldsymbol{x}) \leq 0$ must be active at the solution. To gain some intuition for this idea, we can say that either the solution is on the boundary imposed by the inequality and we must use its KKT multiplier to influence the solution to $\boldsymbol{x}$, or the inequality has no influence on the solution and we represent this by zeroing out its KKT multiplier.

The properties that the gradient of the generalized Lagrangian is zero, all constraints on both $\boldsymbol{x}$ and the KKT multipliers are satisfied, and $\boldsymbol{\alpha} \odot \boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}$ are called the Karush-Kuhn-Tucker (KKT) conditions (Karush, 1939; Kuhn and Tucker, 1951). Together, these properties describe the optimal points of constrained optimization problems.

For more information about the KKT approach, see Nocedal and Wright (2006).

4.5 Example: Linear Least Squares

Suppose we want to find the value of $\boldsymbol{x}$ that minimizes

$$f(\boldsymbol{x}) = \frac{1}{2}||\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}||_2^2. \tag{4.21}$$

There are specialized linear algebra algorithms that can solve this problem efficiently. However, we can also explore how to solve it using gradient-based optimization as a simple example of how these techniques work.

First, we need to obtain the gradient:

$$\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) = \boldsymbol{A}^\top (\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}) = \boldsymbol{A}^\top \boldsymbol{A}\boldsymbol{x} - \boldsymbol{A}^\top \boldsymbol{b}. \tag{4.22}$$

We can then follow this gradient downhill, taking small steps. See Algorithm 4.1 for details.

Algorithm 4.1 An algorithm to minimize $f(\boldsymbol{x}) = \frac{1}{2}||\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}||_2^2$ with respect to $\boldsymbol{x}$ using gradient descent.

Set the step size (ϵ) and tolerance (δ) to small, positive numbers.
while $||\boldsymbol{A}^\top \boldsymbol{A}\boldsymbol{x} - \boldsymbol{A}^\top \boldsymbol{b}||_2 > \delta$ **do**
  $\boldsymbol{x} \leftarrow \boldsymbol{x} - \epsilon \left(\boldsymbol{A}^\top \boldsymbol{A}\boldsymbol{x} - \boldsymbol{A}^\top \boldsymbol{b}\right)$
end while

One can also solve this problem using Newton's method. In this case, because the true function is quadratic, the quadratic approximation employed by Newton's method is exact, and the algorithm converges to the global minimum in a single step.

Now suppose we wish to minimize the same function, but subject to the constraint $\boldsymbol{x}^\top \boldsymbol{x} \leq 1$. To do so, we introduce the Lagrangian

$$L(\boldsymbol{x}, \lambda) = f(\boldsymbol{x}) + \lambda \left(\boldsymbol{x}^\top \boldsymbol{x} - 1\right). \tag{4.23}$$

We can now solve the problem

$$\min_{\boldsymbol{x}} \max_{\lambda, \lambda \geq 0} L(\boldsymbol{x}, \lambda). \tag{4.24}$$

The smallest-norm solution to the unconstrained least squares problem may be found using the Moore-Penrose pseudoinverse: $\boldsymbol{x} = \boldsymbol{A}^+ \boldsymbol{b}$. If this point is feasible, then it is the solution to the constrained problem. Otherwise, we must find a

solution where the constraint is active. By differentiating the Lagrangian with respect to $\boldsymbol{x}$, we obtain the equation

$$\boldsymbol{A}^\top \boldsymbol{A}\boldsymbol{x} - \boldsymbol{A}^\top \boldsymbol{b} + 2\lambda \boldsymbol{x} = 0. \tag{4.25}$$

This tells us that the solution will take the form

$$\boldsymbol{x} = (\boldsymbol{A}^\top \boldsymbol{A} + 2\lambda \boldsymbol{I})^{-1} \boldsymbol{A}^\top \boldsymbol{b}. \tag{4.26}$$

The magnitude of λ must be chosen such that the result obeys the constraint. We can find this value by performing gradient ascent on λ. To do so, observe

$$\frac{\partial}{\partial \lambda} L(\boldsymbol{x}, \lambda) = \boldsymbol{x}^\top \boldsymbol{x} - 1. \tag{4.27}$$

When the norm of $\boldsymbol{x}$ exceeds 1, this derivative is positive, so to follow the derivative uphill and increase the Lagrangian with respect to λ, we increase λ. Because the coefficient on the $\boldsymbol{x}^\top \boldsymbol{x}$ penalty has increased, solving the linear equation for $\boldsymbol{x}$ will now yield a solution with smaller norm. The process of solving the linear equation and adjusting λ continues until $\boldsymbol{x}$ has the correct norm and the derivative on λ is 0.

This concludes the mathematical preliminaries that we use to develop machine learning algorithms. We are now ready to build and analyze some full-fledged learning systems.