Machine Learning Handbook

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Table of Contents

Preface: A starting example with linear regression

Machine learning involves a broad range of techniques for learning from data; a central goal — and the one we largely discuss in this handbook — is prediction. Many learning techniques are centered around learning a function $f : \mathbb{R}^d \to \mathbb{R}$ that inputs attributes or features about an item, and produces an output prediction about that item. For example, consider a setting where you would like to guess or predict the price of a house based on information about that house. You might have features such as its age, the size of the house and of course distance to the nearest bakery. Without any previous examples of house costs, i.e., without any data, it might be hard to guess this price. However, imagine you are given a set of house features and the corresponding selling costs, for houses that sold this year. Let $\mathbf{x} \in \mathbb{R}^d$ be a vector of the features for a house, in this case $\mathbf{x} = [x_1\ x_2\ x_3]$ =[age, size, distance_to_bakery] and the target $y =$ price. If we have 10 examples or instances of previous house prices, we have a dataset: $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_{10}, y_{10})$, where $(\mathbf{x}_i, y_i)$ is the feature-price pair for the ith house in your set of instances. A natural goal is to find a function f that accurately recreates the data, i.e., so that the difference between $f(\mathbf{x}_i)$ and y_i is small for each house.

We can formalize this as an optimization problem. Imagine we have some space of possible functions, $\mathcal{H}$, from which we can select our function f. In this simplest case, let us imagine that the function is linear: $f(\mathbf{x}) = w_0 + x_1 w_1 + x_2 w_2 + x_3 w_3$ for any $\mathbf{w} = [w_0\ w_1\ w_2\ w_3] \in \mathbb{R}^d$ where w_0 is the intercept of the linear function. We can try to find a function from the class of linear functions that minimizes these squared differences

$$\min_{f \in \mathcal{H}} \sum_{i=1}^{10} (f(\mathbf{x}_i) - y_i)^2$$

As we will see later in Chapter 4, this optimization problem is simple to solve for linear functions. The procedure involves explicitly writing the optimization in terms of the parameters $\mathbf{w}$ and solving for the optimal $\mathbf{w}$ that makes the differences as small as possible

$$\begin{aligned} \text{Err}(\mathbf{w}) &= \sum_{i=1}^{10} (f(\mathbf{x}_i) - y_i)^2 \\ &= \sum_{i=1}^{10} \left(w_0 + \sum_{j=1}^{d} w_j x_{ij} - y_i \right)^2 . \end{aligned}$$

We can take the derivative of this error function, and set it to zero to find a stationary point (in this case a global minimum). The solution is a straight line that tries to best fit the observed targets y. A simple illustration of such a function, for only one attribute, is depicted in Figure 1.

Once we have this function, when we see a new house, we hope that it is similar enough to the previous houses so that this function adequately predicts its house price. The learned function f interpolates between these 10 points to predict on unseen points. But, a natural question is, did we interpolate well and is the learned f going to produce an accurate

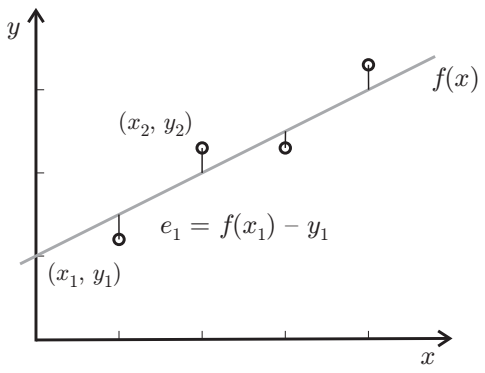


Figure 1: An example of a linear regression fitting on data set $\mathcal{D} = \{(1, 1.2), (2, 2.3), (3, 2.3), (4, 3.3)\}$. *The task of the optimization process is to find the best linear function* $f(x) = w_0 + w_1 x$ *so that the sum of squared errors* $e_1^2 + e_2^2 + e_3^2 + e_4^2$ *is minimized.*

prediction on new houses? If you want to use this learned function f in practice, you want to have such a characterization.

In the agnostic development above, it is difficult to answer such questions. We can make intuitive modifications that we hope will provide more accurate predictions, like extending the class of functions to complex non-linear functions. But, these functional modifications still do not help characterize accuracy of the prediction on new houses. Rather, what we are missing is a notion of confidence. How confident are we in the predictions? Did we see enough previous houses to be confident about this prediction? What is the source of variability? How do we deal with variability? All these types of questions require a probabilistic treatment.

In this handbook, we start by providing an introduction to probability, to provide a base for dealing with uncertainty in machine learning. We then return to learning these functions, once we have the probabilistic tools to better understand how to approach the answers to these questions. Much of the required mathematical background will involve basic understanding of probability and optimization; this handbook will attempt to provide most of that required background throughout.

Chapter 1

Introduction to Probabilistic Modeling

Modeling the world around us and making predictions about the occurrence of events is a multidisciplinary endeavor standing on the solid foundations of probability theory, statistics, and computer science. Although intertwined in the process of modeling, these fields have relatively discernible roles and can be, to a degree, studied individually. Probability theory brings the mathematical infrastructure, firmly grounded in its axioms, for manipulating probabilities and equips us with a broad range of models with well-understood theoretical properties. Statistics contributes frameworks to formulate inference and the process of narrowing down the model space based on the observed data and our experience in order to find, and then analyze, solutions. Computer science provides us with theories, algorithms, and software to manage the data, compute the solutions, and study the relationship between solutions and available resources (time, space, computer architecture, etc.). As such, these three disciplines form the core quantitative framework for all of empirical science and beyond.

Probability theory and statistics have a relatively long history; the formal origins of both can be traced to the 17^{th} century. Probability theory was developed out of efforts to understand games of chance and gambling. The correspondence between Blaise Pascal and Pierre de Fermat in 1654 serves as the oldest record of modern probability theory. Statistics, on the other hand, originated from data collection initiatives and attempts to understand trends in the society (e.g., manufacturing, mortality causes, value of land) and political affairs (e.g., public revenues, taxation, armies). The two disciplines started to merge in the 18^{th} century with the use of data for inferential purposes in astronomy, geography, and social sciences. The increased complexity of models and availability of data in the 19^{th} century emphasized the importance of computing machines. This contributed to establishing the foundations of the field of computer science in the 20^{th} century, which is generally attributed to the introduction of the von Neumann architecture and formalization of the concept of an algorithm. The convergence of the three disciplines has now reached the status of a principled theory of probabilistic inference with widespread applications in science, business, medicine, military, political campaigns, etc. Interestingly, various other disciplines have also contributed to the core of probabilistic modeling. Concepts such as a Boltzmann distribution, a genetic algorithm, or a neural network illustrate the influence of physics, biology, psychology, and engineering.

We will refer to the process of modeling, inference, and decision making based on probabilistic models as *probabilistic reasoning* or reasoning under uncertainty. Some form of reasoning under uncertainty is a necessary component of everyday life. When driving, for example, we often make decisions based on our expectations about which way would be best to take. While these situations do not usually involve an explicit use of probabilities and probabilistic models, an intelligent driverless car such as Google Chauffeur must make use

of them. And so must a spam detection software in an email client, a credit card fraud detection system, or an algorithm that infers whether a particular genetic mutation will result in disease. Therefore, we first need to understand the concept of probability and then introduce a formal theory to incorporate evidence (e.g., data collected from instruments) in order to make good decisions in a range of situations. At a basic level, probabilities are used to quantify the chance of the occurrence of events. As Jacob Bernoulli brilliantly put it in his work *The Art of Conjecturing* (1713), "[p]robability, [...] is the degree of certainty, and it differs from the latter as a part differs from the whole". He later adds, "To make a conjecture [prediction] about something is the same as to measure its probability. Therefore, we define the art of conjecturing [science of prediction] or stochastics, as the art of measuring probabilities of things as accurately as possible, to the end that, in judgements and actions, we may always choose or follow that which has been found to be better, more satisfactory, safer, or more carefully considered." The techniques of probabilistic modeling formalize many intuitive concepts. In a nutshell, they provide toolkits for rigorous mathematical analysis and inference, often in the presence of evidence, about events influenced by factors that we either do not fully understand or have no control of.

To provide a quick insight into the concept of uncertainty and modeling, consider rolling a fair six-sided die. We could accurately predict, or so we think, the outcome of a roll if we carefully incorporated the initial position, force, friction, shape defects, and other physical factors and then executed the experiment. But the physical laws may not be known, they can be difficult to incorporate or such actions may not even be allowed by the rules of the experiment. Thus, it is practically useful to simply assume that each outcome is equally likely; in fact, if we rolled the die many times, we would indeed observe that each number is observed roughly equally. Assigning an equal chance (probability) to each outcome of the roll of a die provides an efficient and elegant way of modeling uncertainties inherent to the experiment.

Another, more realistic example in which collecting data provides a basis for simple probabilistic modeling is a situation of driving to work every day and predicting how long it will take us to reach the destination tomorrow. If we recorded the "time to work" for a few months we would observe that trips generally took different times depending on many internal (e.g., preferred speed for the day) and also external factors (e.g., weather, road works, encountering a slow driver). While these events, if known, could be used to predict the exact duration of the commute, it is unrealistic to expect to have full information. Therefore, it is useful to provide ways of aggregating external factors via collecting data over a period of time and providing the distribution of the commute time. Such a distribution, in the absence of any other information, would then facilitate reasoning about events such as making it on time to an important meeting at 9 am. One way of using the recorded data is to create histograms and calculate percentiles. Another would be to estimate the parameters of some mathematical function that fits the data well. Both approaches are illustrated in Figure 1.1.

As the examples above suggest, the techniques of probabilistic modeling provide a formalism for dealing with repetitive "experiments" influenced by a number of external factors over which we have little control or knowledge. However, we shall see later that probabilities need not be assigned only to events that repeat, but to any event in general. As long as they are assigned according to the formal axioms of probability, we can make inferences because the mathematical formalism does not depend on how the probabilities are assigned.

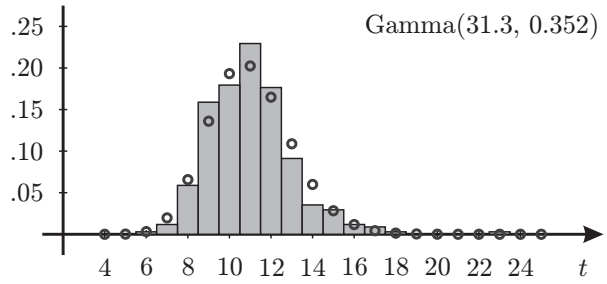


Figure 1.1: A histogram of recordings of the commute time (in minutes) to work. The data set contains 340 measurements collected over one year, for a distance of roughly 3.1 miles. The data was modeled using a gamma family of probability distributions, with the particular location and scale parameters estimated from the raw data. The values of the gamma distribution are shown as dark circles. Although it might seem that fitting the data using a gamma distribution brings little value in this one-dimensional situation, this approach is far superior on high-dimensional data where the number of bins in a multidimensional histogram can be orders of magnitude larger than the data set size.

This provides us an opportunity to incorporate our assumptions and existing knowledge into modeling, including the subjective assessments (beliefs) about occurrence of non-repetitive events. But let us start from the beginning.

1.1 Probability Theory

Probability theory can be seen as a branch of mathematics that deals with set functions. At the heart of probability theory is the concept of an *experiment*. An experiment can be the process of tossing a coin, rolling a die, checking the temperature tomorrow or figuring out the location of one's keys. When carried out, each experiment has an *outcome*, which is an element "drawn" from a set of predefined options, potentially infinite in size. The outcome of a roll of a die is a number between one and six; the temperature tomorrow might be a real number; the outcome of the location of one's keys can be a discrete set of places such as a kitchen table, under a couch, in office etc. In many ways, the main goal of probabilistic modeling is to formulate a particular question or a hypothesis pertaining to the physical world as an experiment, collect the data, and then construct a model. Once a model is created, we can compute quantitative measures of sets of outcomes we are interested in and assess the confidence we should have in these measures.

1.1.1 Axioms of probability

We start by introducing the *axioms of probability*. Let the *sample space* (Ω) be a non-empty set of outcomes of the experiment and the *event space* ($\mathcal{A}$) be a non-empty set of subsets of Ω such that

1. $A \in \mathcal{A} \quad \Rightarrow \quad A^c \in \mathcal{A}$
2. $A_1, A_2, \ldots \in \mathcal{A} \quad \Rightarrow \quad \bigcup_{i=1}^{\infty} A_i \in \mathcal{A}$

where A and all A_i's are *events*, and A^c is the complement of A; i.e., $A^c = \Omega - A$. If both conditions hold, $\mathcal{A}$ is called a sigma field, or sigma algebra, and is a set of so-called measurable events.[1] The tuple $(\Omega, \mathcal{A})$ is then called a *measurable space*.

It is important to emphasize that the definition of sigma field requires that $\mathcal{A}$ be closed under both finite and countably infinite number of basic set operations (union, intersection, complementation and set difference). The operations union and complementation are in the definition. For intersection, we can use De Morgan's laws: $\cup A_i = (\cap A_i^c)^c$ and $\cap A_i = (\cup A_i^c)^c$. Any intersection of sets in $\mathcal{A}$ must again be in $\mathcal{A}$ because $\mathcal{A}$ is closed under union and complementation. Therefore, a sigma field is also closed under intersection. Similarly for set difference, we can write $A_1 - A_2 = (A_1 \cap A_2)^c \cap A_1$, which then implies $A_1 - A_2 \in \mathcal{A}$. Because $\mathcal{A}$ is non-empty, we observe that all the above conditions imply that $\Omega \in \mathcal{A}$ and $\emptyset \in \mathcal{A}$, where $\emptyset$ is the empty set.

Let $(\Omega, \mathcal{A})$ be a measurable space. Any function $P : \mathcal{A} \to [0, 1]$ where

1. $P(\Omega) = 1$
2. $A_1, A_2, \ldots \in \mathcal{A},\ A_i \cap A_j = \emptyset\ \forall i, j \quad \Rightarrow \quad P(\cup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} P(A_i)$

is called a *probability measure* or a *probability distribution* and is said to satisfy the axioms of probability.[2] The tuple $(\Omega, \mathcal{A}, P)$ is called the *probability space*.

The beauty of these axioms lies in their compactness and elegance. Many useful expressions can be derived from the axioms of probability. For example, it is obvious that $P(\emptyset) = 0$ or $P(A^c) = 1 - P(A)$. Similarly, closure under infinite unions of disjoint sets (σ-additivity) implies finite closure (additivity), because the remaining sets can be set to the empty set $\emptyset$: $\forall A_1, A_2 \in \mathcal{A}$ with $A_1 \cap A_2 = \emptyset$, set $A_i = \emptyset$ for $i > 2$ to get $P(A_1 \cup A_2) = P(\cup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} P(A_i) = P(A_1) + P(A_2)$. Another formula that is particularly important can be derived by considering a *partition* of the sample space; i.e., a set of k non-overlapping sets $\{B_i\}_{i=1}^k$ such that $\Omega = \cup_{i=1}^k B_i$. That is, if A is any set in Ω and if $\{B_i\}_{i=1}^k$ is a partition of Ω it follows that

$$\begin{aligned} P(A) &= P(A \cap \Omega) \\ &= P\left(A \cap \left(\cup_{i=1}^k B_i\right)\right) \\ &= P\left(\cup_{i=1}^k (A \cap B_i)\right) \\ &= \sum_{i=1}^k P\left(A \cap B_i\right), \end{aligned} \tag{1.1}$$

where the last line followed from the axioms of probability. We will refer to this expression as the *sum rule*. Another important expression, shown here without a derivation, is that $P(A \cup B) = P(A) + P(B) - P(A \cap B)$.

It is convenient to separately consider discrete (countable) and continuous (uncountable) sample spaces. A roll of a die draws numbers from a finite space $\Omega = \{1, 2, 3, 4, 5, 6\}$. For finite and other countable sample spaces (e.g., the set of integers $\mathbb{Z}$), $\mathcal{A}$ is usually the power

[1] This terminology is due to historical reasons; so though it sounds complex, one can simply think of a sigma field as the set of events to which we can assign probabilities.

[2] It seems intuitive that the second condition could be replaced with a union of finite sets (the simpler requirement of additivity rather than σ-additivity). However, for sigma fields, closure under *finite* unions may not result in closure under *infinite* unions.

set $\mathcal{P}(\Omega)$. An example of continuous sample space is the set of real numbers $\mathbb{R}$. As we shall see later, for uncountable spaces, $\mathcal{A}$ must be a proper subset of $\mathcal{P}(\Omega)$; i.e., $\mathcal{A} \subset \mathcal{P}(\Omega)$, because there exist sets over which one cannot integrate. Technically, sample spaces can also be mixed; e.g., $\Omega = [0,1] \cup \{2\}$ or $\Omega = [0,1] \times \{0,1\}$, but we will not see many of such sets here. The space $\Omega = [0,1] \times \{0,1\}$ is also said to be multidimensional because Ω is a Cartesian product of multiple sets, here $[0,1]$ and $\{0,1\}$. However, the main consideration at this stage will be the distinction between discrete and continuous sample spaces that will give rise to discrete and continuous probability distributions, respectively, and lead to a distinct mathematical treatment.

Owing to many constraints in defining the distribution function P, it is clear that it cannot be chosen arbitrarily. For example, if $\Omega = [0,1]$ and $P([0, \frac{1}{2})) = \frac{1}{2}$, we cannot arbitrarily assign $P([\frac{1}{2}, 1]) = \frac{1}{3}$ because probabilities of complement sets must sum to one. It turns out, in practice it is easier to define P indirectly, by selecting a probability mass function or a probability density function. These functions are defined directly on the sample space where we have fewer restrictions to be concerned with compared to the event space. We address these two ways of defining probability distributions next.

1.1.2 Probability mass functions

Let Ω be a discrete (finite or countably infinite) sample space and $\mathcal{A} = \mathcal{P}(\Omega)$. A function $p : \Omega \to [0,1]$ is called a *probability mass function* (pmf) if

$$\sum_{\omega \in \Omega} p(\omega) = 1.$$

The probability of any event $A \in \mathcal{A}$ is defined as

$$P(A) = \sum_{\omega \in A} p(\omega).$$

It is straightforward to verify that P satisfies the axioms of probability and, thus, is a probability distribution.

Example 1: Consider a roll of a fair six-sided die; i.e., $\Omega = \{1,2,3,4,5,6\}$, and the event space $\mathcal{A} = \mathcal{P}(\Omega)$. What is the probability that the outcome is a number greater than 4?

First, because the die is fair, we know that $p(\omega) = \frac{1}{6}$ for $\forall \omega \in \Omega$. Now, let A be an event in $\mathcal{A}$ that the outcome is greater than 4; i.e., $A = \{5,6\}$. Thus,

$$P(A) = \sum_{\omega \in A} p(\omega) = \frac{1}{3}.$$

It is important to note that P is defined on the elements of $\mathcal{A}$, whereas p is defined on the elements of Ω. That is, $P(\{1\}) = p(1)$, $P(\{2\}) = p(2)$, $P(\{1,2\}) = p(1) + p(2)$, etc. □

In discrete cases, $P(\{\omega\}) = p(\omega)$ for every $\omega \in \Omega$, and the probability of a set is always equal to the sum of probabilities of individual elements. We can define a discrete probability space by providing the tuple $(\Omega, \mathcal{A}, P)$, but it is often much simpler to define P indirectly by assuming that $\mathcal{A} = \mathcal{P}(\Omega)$ and providing a probability mass function p. In this case we say that the probability measure P is induced by a pmf p. In fact, we rarely define $(\Omega, \mathcal{A}, P)$ directly.

A few useful pmfs

Let us now look at some families of functions that are often used to induce discrete probability distributions. This is by no means a comprehensive review of the subject; we shall simply focus on a few basic concepts and will later introduce other distributions as needed. For simplicity, we will often refer to both pmfs and probability distributions they induce as distribution functions.

The *Bernoulli distribution* derives from the concept of a Bernoulli trial, an experiment that has two possible outcomes: success and failure. In a Bernoulli trial, a success occurs with probability α and, thus, failure occurs with probability $1-\alpha$. A toss of a coin (heads/tails), a basketball game (win/loss), or a roll of a die (even/odd) can all be seen as Bernoulli trials. We model this distribution by setting a sample space to two elements and defining the probability of one of them as α. More specifically, $\Omega = \{\text{success}, \text{failure}\}$ and

$$p(\omega) = \begin{cases} \alpha & \omega = \text{success} \\ 1-\alpha & \omega = \text{failure} \end{cases}$$

where $\alpha \in (0,1)$ is a parameter. If we take instead that $\Omega = \{0,1\}$, we can compactly write the Bernoulli distribution as $p(k) = \alpha^k \cdot (1-\alpha)^{1-k}$ for $k \in \Omega$. Here we replaced ω with k, which is a more common notation when the sample space is comprised of integers.

To be precise, the Bernoulli distribution as presented above is actually a family of discrete probability distributions, one for each α. We shall refer to each such distribution as Bernoulli(α). However, we do not need to concern ourselves with semantics because the correct interpretation of a family vs. individual distributions will usually be clear from the context.

The *Binomial distribution* is used to describe a sequence of n independent and identically distributed (i.i.d.) Bernoulli trials. At each value k in the sample space the distribution gives the probability that the success happened exactly k times out of n trials, where of course $0 \leq k \leq n$. More formally, given $\Omega = \{0, 1, \ldots, n\}$, for $\forall k \in \Omega$ the binomial pmf is defined as

$$p(k) = \binom{n}{k} \alpha^k (1-\alpha)^{n-k},$$

where $\alpha \in (0,1)$, as before, is the parameter indicating the probability of success in a single trial. Here, the binomial coefficient

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}$$

enumerates all ways in which one can pick k elements from a list of n elements (e.g., there are 3 different ways in which one can pick $k = 2$ elements from a group of $n = 3$ elements). We will refer to a binomial distribution with parameters n and α as Binomial(n, α). The experiment leading to a binomial distribution can be generalized to a situation with more than two possible outcomes. This experiment results in a multidimensional probability mass function (one dimension per possible outcome) called the multinomial distribution.

The *Poisson distribution* can be derived as a limit of the binomial distribution as $n \to \infty$ with a fixed expected number of successes (λ). Here, $\Omega = \{0, 1, \ldots\}$ and for $\forall k \in \Omega$

$$p(k) = \frac{\lambda^k e^{-\lambda}}{k!},$$

where $\lambda \in (0, \infty)$ is a parameter (the relationship with the binomial distribution can be obtained by taking $\alpha = \lambda/n$). The Poisson distribution is often used to model counts of events occurring sequentially and independently but with a fixed average (λ) in a particular time interval. Unlike the previous two distributions, Poisson(λ) is defined over an infinite sample space, but still countable.

The *geometric distribution* is also used to model a sequence of independent Bernoulli trials with the probability of success α. At each point $k \in \Omega$, it gives the probability that the first success occurs exactly in the k-th trial. Here, $\Omega = \{1, 2, \ldots\}$ and for $\forall k \in \Omega$

$$p(k) = (1 - \alpha)^{k-1}\alpha,$$

where $\alpha \in (0, 1)$ is a parameter. The geometric distribution, Geometric(α), is defined over an infinite sample space; i.e., $\Omega = \mathbb{N}$.

For the *hypergeometric distribution*, consider a finite population of N elements of two types (e.g., success and failure), K of which are of one type (e.g., success). The experiment consists of drawing n elements, without replacement, from this population such that the elements remaining in the population are equiprobable in terms of being selected in the next draw. The probability of drawing k successes out of n trials can be described as

$$p(k) = \frac{\binom{K}{k} \cdot \binom{N-K}{n-k}}{\binom{N}{n}},$$

where $0 \leq n \leq N$ and $k \leq n$. The hypergeometric distribution is intimately related to the binomial distribution where the elements are drawn with replacement ($\alpha = K/N$). There, the probability of drawing a success does not change in subsequent trials. We will refer to the hypergeometric distribution as Hypergeometric(n, N, K).

The *uniform distribution* for discrete sample spaces is defined over a finite set of outcomes each of which is equally likely to occur. Here we can set $\Omega = \{1, \ldots, n\}$; then for $\forall k \in \Omega$

$$p(k) = \frac{1}{n}.$$

The uniform distribution does not contain parameters; it is defined by the size of the sample space. We refer to this distribution as Uniform(n). We will see later that the uniform distribution can also be defined over finite intervals in continuous spaces.

All of the functions above satisfy the definition of a probability mass function, which we can verify by summing over all possible outcomes in the sample space. Four examples are shown in Figure 1.2.

In general, for discrete spaces, we can assign probabilities to outcomes quite freely. For example, one could have a table of 365 values between zero and one for the probability of a birthday falling on each day, as long as the probabilities sum to 1. We will see that for continuous spaces it is more difficult to define consistent probabilities and we will often restrict ourselves to a limited set of known distributions.

1.1.3 Probability density functions

We shall see soon that the treatment of continuous probability spaces is analogous to that of discrete spaces, with probability density functions replacing probability mass functions and integrals replacing sums. Mathematically, however, there are fundamental differences

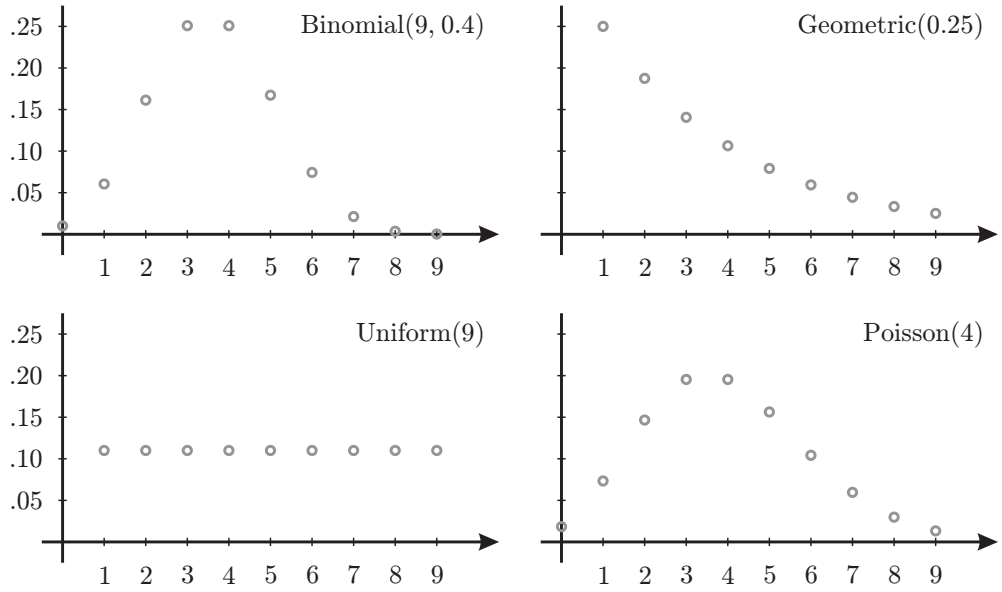


Figure 1.2: Four discrete probability mass functions.

between the two situations which we should keep in mind whenever working with continuous spaces. The main obstacle in generalizing the theory to uncountable sample spaces lies in addressing mathematical nuances involving infinitesimal calculus, the countable nature of a sigma field, and limitations of the definition of integrals. For example, there exist sets over which we cannot integrate and thus the set of events $\mathcal{A}$ cannot be the power set of any uncountable set (e.g., $\mathbb{R}$). It is therefore necessary to define an adequate event space which would be applicable to a vast majority of practically important situations.

To illustrate the treatment of continuous spaces, let us for simplicity take that $\Omega = \mathbb{R}$ and define the Borel field. The Borel field on $\mathbb{R}$, denoted by $\mathcal{B}(\mathbb{R})$, is a set that contains all points in $\mathbb{R}$, all open, semi-open and closed intervals in $\mathbb{R}$, as well as sets that can be obtained by a countable number of basic set operations on them. By definition, $\mathcal{B}(\mathbb{R})$ is a sigma field; $\mathcal{B}(\mathbb{R})$ is an uncountably infinite set, but still smaller than $\mathcal{P}(\mathbb{R})$. The construction of subsets of $\mathbb{R}$ that are not in $\mathcal{B}(\mathbb{R})$ is difficult and only of theoretical importance (e.g., Vitali sets), but nevertheless, the use of $\mathcal{P}(\mathbb{R})$ as the event space would lead to a flawed theory. Therefore, when discussing probability distributions over continuous sample spaces, we will usually take $\Omega = \mathbb{R}$ to be the sample space and implicitly consider $\mathcal{B}(\mathbb{R})$ to be the event space $\mathcal{A}$.

Let now Ω be a continuous sample space and $\mathcal{A} = \mathcal{B}(\Omega)$. A function $p : \Omega \to [0, \infty)$ is called a *probability density function* (pdf) if

$$\int_{\Omega} p(\omega) d\omega = 1.$$

The probability of an event $A \in \mathcal{B}(\Omega)$ is defined as

$$P(A) = \int_{A} p(\omega) d\omega.$$

There are a few mathematical nuances associated with this definition. First, interestingly, the standard Riemann integration does not work for some sets in the Borel field (e.g.,

how would you integrate over the set of rational or irrational numbers within $[0, 1]$ for any pdf?). For that reason, probability density functions are formally defined using Lebesgue integration which allows us to integrate over all sets in $\mathcal{B}(\Omega)$. Luckily, Riemann integration, when possible, provides identical results as Lebesgue's integrals; thus, it will suffice to use Riemann integration in all situations of our interest.

Second, we mentioned before for pmfs that the probability of a singleton event $\{\omega\}$ is the value of the pmf at the sample point ω; i.e., $P(\{\omega\}) = p(\omega)$. In contrast, the value of a pdf at point ω is not a probability; it can actually be greater than 1. The probability at any single point, but also over any finite or countably infinite set is 0 (i.e., they constitute a set of measure zero). One way to think about the probabilities in continuous spaces is to look at small intervals $A = [x, x + \Delta x]$ as

$$\begin{aligned} P(A) &= \int_x^{x+\Delta x} p(\omega) d\omega \\ &\approx p(x)\Delta x. \end{aligned}$$

Here, a potentially large value of the density function is compensated by the small interval Δx to result in a number between 0 and 1.

A few useful pdfs

Some important probability density functions are reviewed below. As before, the sample space will be defined for each distribution and the Borel field will be implicitly assumed as the event space.

The *uniform distribution* is defined by an equal value of a probability density function over a finite interval in $\mathbb{R}$. Thus, for $\Omega = [a, b]$ the uniform probability density function $\forall \omega \in [a, b]$ is defined as

$$p(\omega) = \frac{1}{b-a}.$$

Note that one can also define Uniform(a, b) by taking $\Omega = \mathbb{R}$ and setting $p(\omega) = 0$ whenever ω is outside of $[a, b]$. This form is convenient because $\Omega = \mathbb{R}$ can then be used consistently for all one-dimensional probability distributions. When we do this, we will refer to the subset of $\mathbb{R}$ where $p(\omega) > 0$ as *support* of the density function.

The *exponential distribution* is defined over a set of non-negative numbers; i.e., $\Omega = [0, \infty)$. Its probability density function is

$$p(\omega) = \lambda e^{-\lambda\omega},$$

where $\lambda > 0$ is a parameter. As before, the sample space can be extended to all real numbers, in which case we would set $p(\omega) = 0$ for $\omega < 0$.

The *Gaussian distribution* or normal distribution is one of the most frequently used probability distributions. It is defined over $\Omega = \mathbb{R}$ as

$$p(\omega) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(\omega-\mu)^2}$$

with two parameters, $\mu \in \mathbb{R}$ and $\sigma > 0$. We will refer to this distribution as Gaussian(μ, σ^2) or $\mathcal{N}(\mu, \sigma^2)$. Both Gaussian and exponential distribution are members of a broader family

Figure 1.3: Selection of a random number (x) from the unit interval $[0, 1]$.

of distributions called the exponential family. We will see a general definition of this family later.

The *lognormal distribution* is a modification a normal distribution. Here, for $\Omega = (0, \infty)$ the lognormal density can be expressed as

$$p(\omega) = \frac{1}{\omega\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(\ln\omega - \mu)^2},$$

where $\mu \in \mathbb{R}$ and $\sigma > 0$ are parameters. We will refer to this distribution as Lognormal(μ, σ^2) or $\ln\mathcal{N}(\mu, \sigma^2)$.

The *Gumbel distribution* belongs to the class of extreme value distributions. Its probability density function is defined on $\Omega = \mathbb{R}$ as

$$p(\omega) = \frac{1}{\beta} e^{-\frac{\omega-\alpha}{\beta}} e^{-e^{-\frac{\omega-\alpha}{\beta}}},$$

where $\alpha \in \mathbb{R}$ is the location parameter and $\beta > 0$ is the scale parameter. We will refer to this distribution as Gumbel(α, β).

The *Pareto distribution* is useful for modeling events with rare occurrences of extreme values. Its probability density function is defined on $\Omega = [\omega_{\min}, \infty)$ as

$$p(\omega) = \frac{\alpha\omega_{\min}}{\omega^{\alpha+1}},$$

where $\alpha > 0$ is a parameter and $\omega_{\min} > 0$ is the minimum allowed value for ω. We will refer to the Pareto distribution as Pareto$(\alpha, \omega_{\min})$. It leads to a scale-free property when $\alpha \in (0, 2]$.

Example 2: Consider selecting a number (x) between 0 and 1 uniformly randomly (Figure 1.3). What is the probability that the number is greater than $\frac{3}{4}$ or lower than $\frac{1}{4}$?

We know that $\Omega = [0, 1]$. We define an event of interest as $A = \left[0, \frac{1}{4}\right) \cup (\frac{3}{4}, 1]$ and calculate its probability as

$$\begin{aligned} P(A) &= \int_0^{1/4} d\omega + \int_{3/4}^{1} d\omega && \triangleright\ p(\omega) = \frac{1}{b-a} = 1 \\ &= \frac{1}{2}. \end{aligned}$$

Because the probability of any individual event in a continuous case is 0, there is no difference in integration if we consider open or closed intervals. □

1.1.4 Multidimensional distributions

It is often convenient to think of the sample space as a multidimensional space. In the discrete case, one can think of the sample space Ω as a multidimensional array or as a d-dimensional tensor (note a matrix is a 2D tensor). That is, $\Omega = \Omega_1 \times \Omega_2 \times \ldots \times \Omega_d$, where Ω_i can be seen as the sample space along dimension i. Then, any function $p : \Omega_1 \times \Omega_2 \times \ldots \times \Omega_d \to [0, 1]$ is called a multidimensional probability mass function if

$$\sum_{\omega_1 \in \Omega_1} \cdots \sum_{\omega_d \in \Omega_d} p\left(\omega_1, \omega_2, \ldots, \omega_d\right) = 1.$$

One example of the multidimensional pmf is the multinomial distribution, which generalizes the binomial distribution to the case when the number of outcomes in any trial is a positive integer $d \geq 2$.

The *multinomial distribution* is used to model a sequence of n independent and identically distributed (i.i.d.) trials with d outcomes. At each point $(k_1, k_2, \ldots, k_d)$ in the sample space, the multinomial pmf provides the probability that the outcome 1 occurred k_1 times, outcome 2 occurred k_2 times, etc. Of course, $0 \leq k_i \leq n$ for $\forall i$ and $\sum_{i=1}^{d} k_i = n$. More formally, given the sample space $\Omega = \{0, 1, \ldots, n\}^d$, the multinomial pmf is defined as

$$p(k_1, k_2, \ldots, k_d) = \begin{cases} \binom{n}{k_1, k_2, \ldots, k_d} \alpha_1^{k_1} \alpha_2^{k_2} \ldots \alpha_d^{k_d} & k_1 + k_2 + \cdots + k_d = n \\ \\ 0 & \text{otherwise} \end{cases}$$

where α_i's are positive coefficients such that $\sum_{i=1}^{d} \alpha_i = 1$. That is, each coefficient α_i gives the probability of outcome i in any trial. The multinomial coefficient

$$\binom{n}{k_1, k_2, \ldots, k_d} = \frac{n!}{k_1! k_2! \cdots k_d!}$$

generalizes the binomial coefficient by enumerating all ways in which one can distribute n balls into d boxes such that the first box contains k_1 balls, the second box k_2 balls, etc. An experiment consisting of n tosses of a fair six-sided die and counting the number of occurrences of each number can be described by a multinomial distribution. Clearly, in this case $\alpha_i = 1/6$, for each $i \in \{1, 2, 3, 4, 5, 6\}$.

In the continuous case, we can think of the sample space as the d-dimensional Euclidean space; i.e., $\Omega = \mathbb{R}^d$ and an event space as $\mathcal{A} = \mathcal{B}(\mathbb{R})^d$. Then, the d-dimensional probability density function can be defined as any function $p : \mathbb{R}^d \to [0, \infty)$ such that

$$\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} p(\omega_1, \omega_2, \ldots, \omega_d) d\omega_1 \cdots d\omega_d = 1.$$

The *multivariate Gaussian distribution* is a generalization of the Gaussian or normal distribution to the d-dimensional case, with $\Omega = \mathbb{R}^d$. It is defined as

$$p(\boldsymbol{\omega}) = \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}|}} \exp\left(-\frac{1}{2}(\boldsymbol{\omega} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{\omega} - \boldsymbol{\mu})\right),$$

with parameters $\boldsymbol{\mu} \in \mathbb{R}^d$ and a positive definite d-by-d matrix $\boldsymbol{\Sigma}$ ($|\boldsymbol{\Sigma}|$ is the determinant of $\boldsymbol{\Sigma}$). We will refer to this distribution as Gaussian$(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ or $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.

1.1.5 Interpretation of probability

There are two opposing philosophical views of probability, an *objectivist* and a *subjectivist* one. Objectivists see probability as a concept rooted in reality. Their scientific method is based on the existence of an underlying true probability for an experiment or a hypothesis in question; this underlying probability then needs to be estimated from data. An objectivist is restricted by the known facts about reality (assuming these facts are agreed upon) and derives from them to estimate probabilities. On the other end of the spectrum is a purely subjectivist view in which probabilities represent an observer's *degree of belief* or *conviction* about the outcome of the experiment. A subjectivist is unrestricted by the agreed upon facts and can express any views about an experiment because probabilities are inherently related to one's perception. The good news is, this long-standing philosophical debate has almost no bearing on the use of probability theory in practice. No matter how probabilities are assigned, and it mostly through a combination of subjective and objective steps, the mechanics of probabilistic manipulations are the same and valid, as long as the assignments adhere to the axioms of probability.

1.2 Random Variables

Until now we operated on relatively simple sample spaces and produced measure functions over sets of outcomes. In many situations, however, we would like to use probabilistic modeling on sets (e.g., a group of people) where elements can be associated with various descriptors. For example, a person may be associated with his/her age, height, citizenship, IQ, or marital status and we may be interested in events related to such descriptors. In other situations, we may be interested in transformations of sample spaces such as those corresponding to digitizing an analog signal from a microphone into a set of integers based on some set of voltage thresholds. The mechanism of a *random variable* facilitates addressing all such situations in a simple, rigorous and unified manner.

A random variable is a variable that, from the observer's point of view, takes values non-deterministically, with generally different preferences for different outcomes. Mathematically, however, it is defined as function that maps one sample space into another, with a few technical caveats we will introduce later. Let us motivate the need for random variables. Consider a probability space $(\Omega, \mathcal{A}, P)$, where Ω is a set of people and let us investigate the probability that a randomly selected person $\omega \in \Omega$ is happy (we may assume we have a diagnostic method to assess any person's status). We start by defining an event A as

$$A = \{\omega \in \Omega : Status(\omega) = \text{happy}\}$$

and simply calculate the probability of this event. This is a perfectly legitimate approach, but it can be much simplified using the random variable mechanism. We first note that, technically, our diagnostic method corresponds to a function $Status : \Omega \to \mathcal{S}$ that maps the sample space Ω to a new binary sample space $\mathcal{S} = \{\text{happy, not happy}\}$. More interestingly, our approach also maps the probability distribution P to a new probability distribution P_{Status} that is defined on some sigma algebra of $\mathcal{S}$; say, $\mathcal{A}_{Status}$ (for the mapping to work as expected, $\mathcal{A}_{Status}$ has to be the power set of $\mathcal{S}$). We can now see that we can calculate $P_{Status}(\{\text{happy}\})$ from the probability of the aforementioned event A; i.e., $P_{Status}(\{\text{happy}\}) = P(A)$. This is a cluttered notation so we may wish to simplify it by using $P(Status = \text{happy})$, where $Status$ is a "random variable".

We will use capital letters $X, Y, \ldots$ to denote random variables (such as *Status*) and lowercase letters $x, y, \ldots$ to indicate elements (such as "happy") of the new spaces $\mathcal{X}, \mathcal{Y} \ldots$ Generally, we will write probabilities as $P(X = x)$, which is a notational relaxation from $P(\{\omega : X(\omega) = x\})$, or $P(X \leq x)$ for $P(\{\omega : X(\omega) \leq x\})$ when the co-domain $\mathcal{X}$ is continuous. We will also refer to the corresponding probability mass or density functions as $p(x)$ or $p_X(x)$ when when we need to be more explicit about the random variable. This will indeed happen when x takes a particular value; say, for $x = 1$, we will write $p_X(1)$. Before we proceed to formally define random variables, we shall look at two illustrative examples.

Example 3: Consecutive tosses of a fair coin. Consider a process of three coin tosses and two random variables, X and Y, defined on the sample space. We define X as the number of heads in the first toss and Y as the number of heads over all three tosses. Our goal is to find the probability spaces that are created after the transformations.

First, $\Omega = \{\text{HHH}, \text{HHT}, \text{HTH}, \text{HTT}, \text{THH}, \text{THT}, \text{TTH}, \text{TTT}\}$ and

ω	HHH	HHT	HTH	HTT	THH	THT	TTH	TTT
$X(\omega)$	1	1	1	1	0	0	0	0
$Y(\omega)$	3	2	2	1	2	1	1	0

Let us only focus on variable Y. Clearly, $Y : \Omega \to \{0, 1, 2, 3\}$ but we also need to find $\mathcal{A}_Y$ and P_Y. To calculate P_Y, a simple approach is to find its pmf $p(y)$. For example, let us calculate $p_Y(2) = P_Y(\{2\})$ as

$$\begin{aligned} P_Y(\{2\}) &= P(Y = 2) \\ &= P(\{\omega : Y(\omega) = 2\}) \\ &= P(\{\text{HHT}, \text{HTH}, \text{THH}\}) \\ &= \frac{3}{8}, \end{aligned}$$

because of the uniform distribution in the original space $(\Omega, \mathcal{A}, P)$. In a similar way, we can calculate that $P(Y = 0) = P(Y = 3) = 1/8$, and that $P(Y = 1) = 3/8$. In this example, we took that $\mathcal{A} = \mathcal{P}(\Omega)$ and $\mathcal{A}_Y = \mathcal{P}(\mathcal{Y})$. As a final note, we mention that all the randomness is defined in the original probability space $(\Omega, \mathcal{A}, P)$ and that the new probability space $(\mathcal{Y}, \mathcal{A}_Y, P_Y)$ simply inherits it through a deterministic transformation.

□

Example 4: Quantization. Consider $(\Omega, \mathcal{A}, P)$ where $\Omega = [0, 1]$, $\mathcal{A} = \mathcal{B}(\Omega)$, and P is induced by a uniform pdf. Define $X : \Omega \to \{0, 1\}$ as

$$X(\omega) = \begin{cases} 0 & \omega \leq 0.5 \\ 1 & \omega > 0.5 \end{cases}$$

and find the transformed probability space.

Technically, we have changed the sample space to $\mathcal{X} = \{0, 1\}$. For an event space $\mathcal{A}_X = \mathcal{P}(\mathcal{X}) = \{\emptyset, \{0\}, \{1\}, \{0, 1\}\}$ we would like to understand the new probability distribution

P_X. We have

$$\begin{aligned} p_X(0) &= P_X(\{0\}) \\ &= P(X = 0) \\ &= P(\{\omega : \omega \in [0, 0.5]\}) \\ &= \frac{1}{2} \end{aligned}$$

and

$$\begin{aligned} p_X(1) &= P_X(\{1\}) \\ &= P(X = 1) \\ &= P(\{\omega : \omega \in (0.5, 1]\}) \\ &= \frac{1}{2} \end{aligned}$$

From here we can easily see that $P_X(\{0, 1\}) = 1$ and $P_X(\emptyset) = 0$, and so P_X is indeed a probability distribution. Again, P_X is naturally defined using P. Thus, we have transformed the probability space $(\Omega, \mathcal{A}, P)$ into $(\mathcal{X}, \mathcal{A}_X, P_X)$.

□

The mapping from a continuous Ω to other continuous samples spaces is slightly more complicated and will be considered later.

1.2.1 Formal definition of random variable

We now formally define a random variable. Given a probability space $(\Omega, \mathcal{A}, P)$, a random variable X is a function $X : \Omega \to \mathcal{X}$ such that for every $A \in \mathcal{B}(\mathcal{X})$ it holds that $\{\omega : X(\omega) \in A\} \in \mathcal{A}$. It follows that

$$P_X(A) = P(\{\omega : X(\omega) \in A\}).$$

It is important to mention that, by default, we defined the event space of a random variable to be the Borel field of $\mathcal{X}$. This is convenient because a Borel field of a countable set Ω is its power set. Thus, we are working with the largest possible event spaces for both discrete and continuous random variables.

Consider now a *discrete random variable* X defined on $(\Omega, \mathcal{A}, P)$. As we can see from the previous examples, the probability distribution for X can be found as

$$\begin{aligned} p(x) &= P_X(\{x\}) \\ &= P(\{\omega : X(\omega) = x\}) \end{aligned}$$

for $\forall x \in \mathcal{X}$. The probability of an event A can be found as

$$\begin{aligned} P_X(A) &= P(\{\omega : X(\omega) \in A\}) \\ &= \sum_{x \in A} p(x) \end{aligned}$$

for $\forall A \subseteq \mathcal{X}$.

The case of *continuous random variables* is more complicated, but reduces to an approach that is similar to that of discrete random variables. Here we first define a *cumulative distribution function* (cdf) as

$$\begin{aligned} F_X(t) &= P_X\left(\{x : x \leq t\}\right) \\ &= P\left(\{\omega : X(\omega) \leq t\}\right) \\ &= P\left(X \leq t\right), \end{aligned}$$

where $P\left(X \leq t\right)$, as before, presents a minor abuse of notation. If the cumulative distribution function is differentiable, the probability density function of a continuous random variable is defined as

$$p\left(x\right) = \left.\frac{dF_X\left(t\right)}{dt}\right|_{t=x}.$$

Alternatively, if $p(x)$ exists, then

$$F_X\left(t\right) = \int_{-\infty}^{t} p\left(x\right) dx,$$

for each $t \in \mathbb{R}$. Our focus will be exclusively on random variables that have their probability density functions; however, for a more general view, we should always keep in mind "if one exists" when referring to pdfs.

The probability that a random variable will take a value from interval $(a, b]$ can now be calculated as

$$\begin{aligned} P_X((a,b]) &= P(a < X \leq b) \\ &= \int_a^b p\left(x\right) dx \\ &= F_X\left(b\right) - F_X\left(a\right), \end{aligned}$$

which follows from the properties of integration.

Suppose now that the random variable X transforms a probability space $(\Omega, \mathcal{A}, P)$ into $(\mathcal{X}, \mathcal{B}(\mathcal{X}), P_X)$. To describe the resulting probability space, we commonly use probability mass and density functions inducing P_X. For example, if P_X is induced by a Gaussian distribution with parameters μ and σ^2, we use

$$X : \mathcal{N}(\mu, \sigma^2) \qquad \text{or} \qquad X \sim \mathcal{N}(\mu, \sigma^2).$$

Both notations indicate that the probability density function for the random variable X is

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}.$$

The Gaussian density implicitly defined that $\mathcal{X} = \mathbb{R}$. This point however is superficial because we can always extend the domain of a density function to $\mathbb{R}$ and set $p(x) = 0$ wherever the original function was not defined.

A group of d random variables $\{X_i\}_{i=1}^d$ defined on the same probability space $(\Omega, \mathcal{A}, P)$ is called a *random vector* or a multivariate (multidimensional) random variable. We have

already seen an example of a random vector provided by random variables (X, Y) in Example 3. A generalization of a random vector to infinite sets is referred to as a *random process* or *stochastic process*; i.e., $\{X_i : i \in \mathcal{T}\}$, where $\mathcal{T}$ is an index set usually interpreted as a set of time indices. In the case of discrete time indices (e.g., $\mathcal{T} = \mathbb{N}$) the random process is called a discrete-time random process; otherwise (e.g., $\mathcal{T} = \mathbb{R}$) it is called a continuous-time random process. There are many models in machine learning that deal with temporally-connected random variables (e.g., autoregressive models for time series, Markov chains, hidden Markov models, dynamic Bayesian networks). The language of random variables, through stochastic processes, nicely enables formalization of these models. Most of these notes, however, will deal with simpler settings only requiring (i.i.d.) multivariate random variables.

1.2.2 Joint and marginal distributions

Let us first look at two discrete random variables X and Y defined on the same probability space $(\Omega, \mathcal{A}, P)$. We define the *joint probability distribution* $p(x, y)$, or when needed $p_{XY}(x, y)$, of X and Y as

$$\begin{aligned} p(x, y) &= P(X = x, Y = y) \\ &= P(\{\omega : X(\omega) = x\} \cap \{\omega : Y(\omega) = y\}). \end{aligned}$$

We can extend this to a d-dimensional random variable $\boldsymbol{X} = (X_1, X_2, \ldots, X_d)$ and define a multidimensional probability mass function as $p(\boldsymbol{x})$ or $p_{\boldsymbol{X}}(\boldsymbol{x})$, where $\boldsymbol{x} = (x_1, x_2, \ldots, x_d)$ is a vector of values, such that each x_i is chosen from some $\mathcal{X}_i$.

A *marginal distribution* is defined for a subset of $\boldsymbol{X} = (X_1, X_2, \ldots, X_d)$ by summing or integrating over the remaining variables. A marginal distribution $p(x_i)$ or $p_{X_i}(x_i)$ is defined as

$$p(x_i) = \sum_{x_1} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_d} p(x_1, \ldots, x_d),$$

where the j-th variable takes values from $\mathcal{X}_j$. The previous equation directly follows from Equation (1.1) and is also referred to as *sum rule*.

In the continuous case, we define a multidimensional cdf as

$$\begin{aligned} F_{\boldsymbol{X}}(\boldsymbol{t}) &= P_{\boldsymbol{X}}(\{\boldsymbol{x} : x_i \leq t_i, i = 1 \ldots d\}) \\ &= P(X_1 \leq t_1, X_2 \leq t_2, \ldots, X_d \leq t_d) \end{aligned}$$

and the probability density function, if it exists, is defined as

$$p(\boldsymbol{x}) = \frac{\partial^d}{\partial t_1 \cdots \partial t_d} F_{\boldsymbol{X}}(t_1, \ldots t_d)\Big|_{\boldsymbol{t}=\boldsymbol{x}}.$$

The marginal density $p_{X_i}(x_i)$ is defined as

$$p(x_i) = \int_{\mathcal{X}_1} \cdots \int_{\mathcal{X}_{i-1}} \int_{\mathcal{X}_{i+1}} \cdots \int_{\mathcal{X}_d} p(\boldsymbol{x})\, dx_1 \cdots dx_{i-1} dx_{i+1} \cdots dx_d$$

If the sample space for each discrete random variable is seen as a countable subset of $\mathbb{R}$, then the probability space for any discrete or continuous d-dimensional random variable $\boldsymbol{X}$ can be defined as $\left(\mathbb{R}^d, \mathcal{B}(\mathbb{R})^d, P_{\boldsymbol{X}}\right)$.

Example 5: Three tosses of a fair coin (again). Consider two random variables from Example 3 and calculate their probability spaces, joint and marginal distributions. Recall X is the number of heads in the first toss and Y is the number of heads over all three tosses.

A joint probability mass function $p(x, y) = P(X = x, Y = y)$ is shown below

		Y			
		0	1	2	3
X	0	$1/8$	$1/4$	$1/8$	0
	1	0	$1/8$	$1/4$	$1/8$

but let us step back for a moment and show how we can calculate it. Let us consider two sets $A = \{\text{HHH, HHT, HTH, HTT}\}$ and $B = \{\text{HHT, HTH, THH}\}$, corresponding to the events that the first toss was heads and that there were exactly two heads over the three tosses, respectively. Now, let us look at the probability of the intersection of A and B

$$\begin{aligned} P(A \cap B) &= P(\{\text{HHT}, \text{HTH}\}) \\ &= \frac{1}{4} \end{aligned}$$

We can represent the probability of the logical statement $X = 1 \wedge Y = 2$ as

$$\begin{aligned} p_{XY}(1, 2) &= P(X = 1, Y = 2) \\ &= P(A \cap B) \\ &= P(\{\text{HHT}, \text{HTH}\}) \\ &= \frac{1}{4}. \end{aligned}$$

The marginal probability distribution can be found in a straightforward way as

$$p(x) = \sum_{y \in \mathcal{Y}} p(x, y),$$

where $\mathcal{Y} = \{0, 1, 2, 3\}$. Thus,

$$\begin{aligned} p_X(0) &= \sum_{y \in \mathcal{Y}} p_{XY}(0, y) \\ &= \frac{1}{2}. \end{aligned}$$

We note for the end that in the discrete case we have $|\mathcal{X}| \cdot |\mathcal{Y}| - 1$ free parameters (because the sum must equal 1) to fully describe the joint distribution $p(x, y)$. Asymptotically, this corresponds to an exponential growth of the number of entries in the table with the number of random variables (d). For example, if $|\mathcal{X}_i| = 2$ for $\forall X_i$, there are $2^d - 1$ free elements in the joint probability distribution. Estimating such distributions from data is intractable and is one form of the *curse of dimensionality*.

□

1.2.3 Conditional distributions

The conditional probability distribution for two random variables X and Y, $p(y|x)$ or $p_{Y|X}(y|x)$, is defined as[3]

$$p(y|x) = \frac{p(x,y)}{p(x)}, \tag{1.2}$$

where $p(x) > 0$. Equation (1.2) now allows us to calculate the posterior probability of an event A, given some observation x, as

$$P(Y \in A|X = x) = \begin{cases} \sum_{y \in A} p(y|x) & Y : \text{discrete} \\ \\ \int_A p(y|x)dy & Y : \text{continuous} \end{cases}$$

Writing $p(x,y) = p(x|y)p(y) = p(y|x)p(x)$ is called the *product rule*. The extension to more than two variables is straightforward. We can write

$$p(x_d|x_1, \ldots, x_{d-1}) = \frac{p(x_1, \ldots, x_d)}{p(x_1, \ldots, x_{d-1})}.$$

By a recursive application of the product rule, we obtain

$$p(x_1, \ldots, x_d) = p(x_1) \prod_{i=2}^{d} p(x_i|x_1, \ldots, x_{i-1}) \tag{1.3}$$

which is referred to as the *chain rule* or *general product rule*. Using the product rule, we can derive *Bayes' rule*:

$$p(x|y) = \frac{p(y|x)p(x)}{p(y)}. \tag{1.4}$$

1.2.4 Independence of random variables

Two random variables are independent if their joint probability distribution can be expressed as

$$p\left(x,y\right) = p(x) \cdot p(y).$$

As before, d random variables are (mutually, jointly) independent if a joint probability distribution of any subset of variables can be expressed as a product of individual (marginal) probability distributions of its components.

Another, different, form of independence can be found even more frequently in probabilistic calculations. It represents independence between variables in the presence of some other random variable (evidence); e.g.,

$$p\left(x,y|z\right) = p(x|z) \cdot p(y|z)$$

and is referred to as *conditional independence*. Interestingly, the two forms of independence are unrelated; i.e., neither one implies the other. We show this in two simple examples from Figure 1.4.

[3]It is straightforward to verify that $p(y|x)$ sums (integrates) to 1 over all values $y \in \mathcal{Y}$, and thus satisfies the conditions of a probability mass (density) function.

A. X and Y are independent, but not conditionally independent given Z

$P(X=1)$
a

$$P(Y=y|X=x) = P(Y=y)$$

for example,

$$P(Y=1|X=x) = b$$
$$P(Y=1) = b$$

X	$P(Y=1\|X)$
0	b
1	b

$$P(Y=y|X=x, Z=z) \neq P(Y=y|Z=z)$$

for example,

$$P(Y=1|X=1, Z=1) = bc/(1-c-b(1-2c))$$
$$P(Y=1|Z=1) = b(1-c-a(1-2c))/d$$
where $d = P(Z=1)$

X	Y	$P(Z=1\|X,Y)$
0	0	c
0	1	$1-c$
1	0	$1-c$
1	1	c

B. X and Z are conditionally independent given Y, but not independent

$P(X=1)$
a

$$P(Z=z|X=x) \neq P(Z=z)$$

for example,

$$P(Z=1|X=1) = d + ce - cd$$
$$P(Z=1) = d + (e-d)(a(c-b)+b)$$

X	$P(Y=1\|X)$
0	b
1	c

$$P(Z=z|X=x, Y=y) = P(Z=z|Y=y)$$

for example,

$$P(Z=1|X=x, Y=1) = e$$
$$P(Z=1|Y=1) = e$$

X	Y	$P(Z=1\|X,Y)$
0	0	d
0	1	e
1	0	d
1	1	e

Figure 1.4: Independence vs. conditional independence using probability distributions involving three binary random variables. Probability distributions are presented using factorization $p(x,y,z) = p(x)p(y|x)p(z|x,y)$, where all constants $a,b,c,d,e \in [0,1]$. (A) Variables X and Y are independent, but not conditionally independent given Z. When $c=0$, $Z = X \oplus Y$, where $\oplus$ is an "exclusive or" operator. (B) Variables X and Z are conditionally independent given Y, but are not independent.

1.2.5 Expectations and moments

Expectations of functions are defined as sums (or integrals) of function values weighted according to the probability mass (or density) function. Given a probability space $(\mathcal{X}, \mathcal{B}(\mathcal{X}), P_X)$, we consider a function $f : \mathcal{X} \to \mathbb{C}$ and define its expectation function as

$$\mathbb{E}\left[f(X)\right] = \begin{cases} \sum_{x \in \mathcal{X}} f(x)p(x) & X : \text{discrete} \\ \\ \int_{\mathcal{X}} f(x)p(x)dx & X : \text{continuous} \end{cases}$$

Note that we use a capital X for the random variable (with $f(X)$ the random variable transformed by f) and lower case x when it is an instance (e.g., $p(x)$ is the probability of a specific outcome). The capital X in $\mathbb{E}\left[f(X)\right]$ also specifies that the summation (integration) is defined over $p(x)$; this will become more important later when we consider multiple random variables. It can happen that $\mathbb{E}\left[f(X)\right] = \pm\infty$; in such cases we say that the expectation does not exist or is not well-defined.[4] For $f(x) = x$, we have a standard expectation $\mathbb{E}\left[X\right] = \sum xp(x)$, or the mean value of X. Using $f(x) = x^k$ results in the k-th moment, $f(x) = \log {}^1\!/_{p(x)}$ gives the well-known entropy function $H(X)$, or differential entropy for continuous random variables, and $f(x) = \left(x - \mathbb{E}\left[X\right]\right)^2$ provides the variance of a random variable X, denoted by $V\left[X\right]$. Interestingly, the probability of some event $A \subseteq \mathcal{X}$[5] can also be expressed in the form of expectation; i.e.,

$$P(A) = \mathbb{E}\left[1(X \in A)\right],$$

where

$$1(t) = \begin{cases} 1 & t \text{ is true} \\ 0 & t \text{ is false} \end{cases} \tag{1.5}$$

is an indicator function. With this, it is possible to express the cumulative distribution function as $F_X(t) = \mathbb{E}[1(X \in (-\infty, t])]$.

Function $f(x)$ inside the expectation can also be complex-valued. For example, $\varphi_X(t) = \mathbb{E}[e^{itX}]$, where i is the imaginary unit, defines the characteristic function of X. The characteristic function is closely related to the inverse Fourier transform of $p(x)$ and is useful in many forms of statistical inference. Several expectation functions are summarized in Table 1.1.

Given two random variables X and Y and a specific value x assigned to X, we define the conditional expectation as

$$\mathbb{E}\left[f(Y)|x\right] = \begin{cases} \sum_{y \in \mathcal{Y}} f(y)p(y|x) & Y : \text{discrete} \\ \\ \int_{\mathcal{Y}} f(y)p(y|x)dy & Y : \text{continuous} \end{cases}$$

[4] There is sometimes disagreement on terminology, and some definitions allow the expected value to be infinite, which, for example, still allows the strong law of large numbers. In that setting, an expectation is not well-defined only if both left and right improper integrals are infinite. For our purposes, this is splitting hairs.

[5] This notation is a bit loose; we should say $A \in \mathcal{B}(\mathcal{X})$ instead of $A \subseteq \mathcal{X}$. We used it to re-emphasize (through this footnote) that some subsets of continuous sets are not measurable.

$f(x)$	Symbol	Name
x	$\mathbb{E}[X]$	Mean
$(x - \mathbb{E}[X])^2$	$V[X]$	Variance
x^k	$\mathbb{E}[X^k]$	k-th moment; $k \in \mathbb{N}$
$(x - \mathbb{E}[X])^k$	$\mathbb{E}[(X - \mathbb{E}[X])^k]$	k-th central moment; $k \in \mathbb{N}$
e^{tx}	$M_X(t)$	Moment generating function
e^{itx}	$\varphi_X(t)$	Characteristic function
$\log \frac{1}{p(x)}$	$H(X)$	(Differential) entropy
$\log \frac{p(x)}{q(x)}$	$D(p\|\|q)$	Kullback-Leibler divergence
$\left(\frac{\partial}{\partial\theta} \log p(x\|\theta)\right)^2$	$\mathcal{I}(\theta)$	Fisher information

Table 1.1: Some important expectation functions $\mathbb{E}[f(X)]$ for a random variable X described by its distribution $p(x)$. Function $q(x)$ in the definition of the Kullback-Leibler divergence is non-negative and must sum (integrate) to 1; i.e., it is a probability distribution itself. The Fisher information is defined for a family of probability distributions specified by a parameter θ. Note that the moment generating function may not exist for some distributions and all values of t; however, the characteristic function always exists, even when the density function does not.

$f(x, y)$	Symbol	Name
$(x - \mathbb{E}[X])(y - \mathbb{E}[Y])$	$\mathrm{Cov}[X, Y]$	Covariance
$\frac{(x-\mathbb{E}[X])(y-\mathbb{E}[Y])}{\sqrt{V[X]V[Y]}}$	$\mathrm{Corr}[X, Y]$	Correlation
$\log \frac{p(x,y)}{p(x)p(y)}$	$I(X;Y)$	Mutual information
$\log \frac{1}{p(x,y)}$	$H(X, Y)$	Joint entropy
$\log \frac{1}{p(x\|y)}$	$H(X\|Y)$	Conditional entropy

Table 1.2: Some important expectation functions $\mathbb{E}[f(X, Y)]$ for two random variables, X and Y, described by their joint distribution $p(x, y)$. Mutual information is sometimes referred to as average mutual information.

where $f : \mathcal{Y} \to \mathbb{C}$ is some function. Again, using $f(y) = y$ results in $\mathbb{E}[Y|x] = \sum yp(y|x)$ or $\mathbb{E}[Y|x] = \int yp(y|x)dy$. We shall see later that under some conditions $\mathbb{E}[Y|x]$ is referred to as the *regression function*. These types of integrals are often seen and evaluated in Bayesian statistics.

For two random variables X and Y we also define

$$\mathbb{E}[f(X,Y)] = \begin{cases} \sum_{x\in\mathcal{X}} \sum_{y\in\mathcal{Y}} f(x,y)p(x,y) & X,Y : \text{discrete} \\ \\ \int_{\mathcal{X}} \int_{\mathcal{Y}} f(x,y)p(x,y)dxdy & X,Y : \text{continuous} \end{cases}$$

Expectations can also be defined over a single variable

$$\mathbb{E}[f(X,y)] = \begin{cases} \sum_{x\in\mathcal{X}} f(x,y)p(x) & X : \text{discrete} \\ \\ \int_{\mathcal{X}} f(x,y)p(x)dx & X : \text{continuous} \end{cases}$$

where $\mathbb{E}[f(X,y)]$ is now a function of y.

We define the covariance function as

$$\begin{aligned} \text{Cov}[X,Y] &= \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])] \\ &= \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y], \end{aligned}$$

with $\text{Cov}[X,X] = V[X]$ being the variance of the random variable X. Similarly, we define a correlation function as

$$\text{Corr}[X,Y] = \frac{\text{Cov}[X,Y]}{\sqrt{V[X] \cdot V[Y]}},$$

which is simply a covariance function normalized by the product of standard deviations. Both covariance and correlation functions have wide applicability in statistics, machine learning, signal processing and many other disciplines. Several important expectations for two random variables are listed in Table 1.2.

Example 6: Three tosses of a fair coin (yet again). Consider two random variables from Examples 3 and 5, and calculate the expectation and variance for both X and Y. Then calculate $\mathbb{E}[Y|X = 0]$.

We start by calculating $\mathbb{E}[X] = 0 \cdot p_X(0) + 1 \cdot p_X(1) = \frac{1}{2}$. Similarly,

$$\begin{aligned} \mathbb{E}[Y] &= \sum_{y=0}^{3} y \cdot p_Y(y) \\ &= p_Y(1) + 2p_Y(2) + 3p_Y(3) \\ &= \frac{3}{2} \end{aligned}$$

The conditional expectation can be found as

$$\begin{aligned} \mathbb{E}[Y|X = 0] &= \sum_{y=0}^{3} y \cdot p_{Y|X}(y|0) \\ &= p_{Y|X}(1|0) + 2p_{Y|X}(2|0) + 3p_{Y|X}(3|0) \\ &= 1 \end{aligned}$$

where $p(y|x) = p(x,y)/p(x)$.

□

In many situations we need to analyze more than two random variables. A simple two-dimensional summary of all pairwise covariance values involving d random variables $X_1, X_2, \ldots, X_d$ is called the covariance matrix. More formally, the covariance matrix is defined as

$$\boldsymbol{\Sigma} = [\Sigma_{ij}]_{i,j=1}^{d}$$

where

$$\begin{aligned}\Sigma_{ij} &= \mathrm{Cov}[X_i, X_j] \\ &= \mathbb{E}\left[(X_i - \mathbb{E}\left[X_i\right])\left(X_j - \mathbb{E}\left[X_j\right]\right)\right]\end{aligned}$$

with the full matrix written as

$$\begin{aligned}\boldsymbol{\Sigma} &= \mathrm{Cov}[\boldsymbol{X}, \boldsymbol{X}] \\ &= \mathbb{E}[(\boldsymbol{X} - \mathbb{E}[\boldsymbol{X}])(\boldsymbol{X} - \mathbb{E}(\boldsymbol{X})^\top] \\ &= \mathbb{E}[\boldsymbol{X}\boldsymbol{X}^\top] - \mathbb{E}[\boldsymbol{X}]\mathbb{E}[\boldsymbol{X}]^\top.\end{aligned}$$

Here, the diagonal elements of a $d \times d$ covariance matrix are individual variance values for each variable X_i and the off-diagonal elements are the covariance values between pairs of variables. The covariance matrix is symmetric and positive semi-definite, i.e., $\boldsymbol{\Sigma} \succeq 0$. We will discuss more about positive semi-definite matrices later in the notes.

Properties of expectations

Here we review, without proofs, some useful properties of expectations. We can generically consider multivariate random variables, $\boldsymbol{X} \in \mathbb{R}^d$ and $\boldsymbol{Y} \in \mathbb{R}^d$, for $d \in \mathbb{N}$, with univariate random variables as a special case. We consider the more general case because it will be useful to start thinking directly in terms of random vectors. For a constant $c \in \mathbb{R}$, it holds that:

1. $\mathbb{E}\left[c\boldsymbol{X}\right] = c\mathbb{E}\left[\boldsymbol{X}\right]$
2. $\mathbb{E}\left[\boldsymbol{X} + \boldsymbol{Y}\right] = \mathbb{E}\left[\boldsymbol{X}\right] + \mathbb{E}\left[\boldsymbol{Y}\right]$
3. $V\left[c\right] = 0$ ▷ the variance of a constant is zero
4. $\mathrm{V}[\boldsymbol{X}] \succeq 0$ (i.e., is positive semi-definite), where for $d = 1$, $\mathrm{V}[\boldsymbol{X}] \geq 0$ is a scalar. Note that $\mathrm{V}[\boldsymbol{X}]$ is shorthand for $\mathrm{Cov}[\boldsymbol{X}, \boldsymbol{X}]$.
5. $\mathrm{V}[c\boldsymbol{X}] = c^2\mathrm{V}[\boldsymbol{X}]$.
6. $\mathrm{Cov}[\boldsymbol{X}, \boldsymbol{Y}] = \mathbb{E}[(\boldsymbol{X} - \mathbb{E}[\boldsymbol{X}])(\boldsymbol{Y} - \mathbb{E}(\boldsymbol{Y})^\top] = \mathbb{E}[\boldsymbol{X}\boldsymbol{Y}^\top] - \mathbb{E}[\boldsymbol{X}]\mathbb{E}[\boldsymbol{Y}]^\top$
7. $\mathrm{Cov}[\boldsymbol{X} + \boldsymbol{Y}] = \mathrm{V}[\boldsymbol{X}] + \mathrm{V}[\boldsymbol{Y}] + 2\mathrm{Cov}[\boldsymbol{X}, \boldsymbol{Y}]$
8. $\mathrm{Cov}[\boldsymbol{X}_1 + \boldsymbol{X}_2 + \ldots + \boldsymbol{X}_m] = \sum_{i=1}^{m}\sum_{j=1}^{m}\mathrm{Cov}[\boldsymbol{X}_i, \boldsymbol{X}_j] = \sum_{i=1}^{m}\mathrm{V}[\boldsymbol{X}_i] + 2\sum_{1 \leq i < j \leq m}\mathrm{Cov}[\boldsymbol{X}_i, \boldsymbol{X}_j]$

In addition, if $\boldsymbol{X}$ and $\boldsymbol{Y}$ are independent random variables of the same dimension, it holds that:

1. $\mathbb{E}[X_i Y_j] = \mathbb{E}[X_i]\,\mathbb{E}[Y_j]$ for all i, j
2. $\mathrm{Cov}[\boldsymbol{X} + \boldsymbol{Y}] = \mathrm{V}[\boldsymbol{X}] + \mathrm{V}[\boldsymbol{Y}]$
3. $\mathrm{Cov}[\boldsymbol{X}, \boldsymbol{Y}] = 0$.

1.2.6 Mixtures of distributions

In previous sections we saw that random variables are often described using particular families of probability distributions. This approach can be generalized by considering mixtures of distributions; i.e., linear combinations of other probability distributions. As before, we shall only consider random variables that have their probability mass or density functions.

Given a set of m probability distributions, $\{p_i(x)\}_{i=1}^m$, a finite mixture distribution function, or *mixture model*, $p(x)$ is defined as

$$p(x) = \sum_{i=1}^{m} w_i p_i(x), \tag{1.6}$$

where $\boldsymbol{w} = (w_1, w_2, \ldots, w_m)$ is a set of non-negative real numbers such that $\sum_{i=1}^m w_i = 1$. We refer to $\boldsymbol{w}$ as mixing coefficients or, sometimes, as mixing probabilities. A linear combination with such coefficients is called a convex combination. It is straightforward to verify that a function defined in this manner is indeed a probability distribution.

Here we will briefly look into the basic expectation functions of the mixture distribution. Suppose $\{X_i\}_{i=1}^m$ is a set of m random variables described by their respective probability distributions $\{p_{X_i}(x)\}_{i=1}^m$. Suppose also that a random variable X is described by a mixture distribution with coefficients $\boldsymbol{w}$ and probability distributions $\{p_{X_i}(x)\}_{i=1}^m$. Then, assuming continuous random variables defined on $\mathbb{R}$, the expectation function is given as

$$\begin{aligned}
\mathbb{E}[f(X)] &= \int_{-\infty}^{+\infty} f(x) p_X(x) dx \\
&= \int_{-\infty}^{+\infty} f(x) \sum_{i=1}^{m} w_i p_{X_i}(x) dx \\
&= \sum_{i=1}^{m} w_i \int_{-\infty}^{+\infty} f(x) p_{X_i}(x) dx \\
&= \sum_{i=1}^{m} w_i \mathbb{E}[f(X_i)].
\end{aligned}$$

We can now apply this formula to obtain the mean, when $f(x) = x$ and the variance, when $f(x) = (x - E[X])^2$, of the random variable X as

$$\mathbb{E}[X] = \sum_{i=1}^{m} w_i \mathbb{E}[X_i],$$

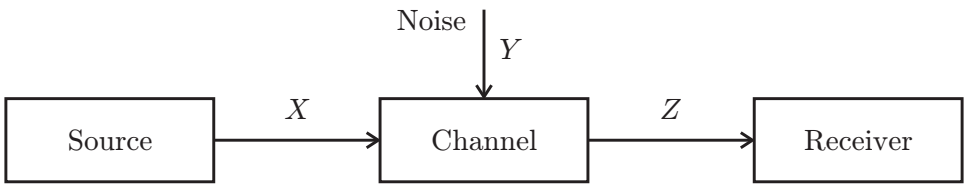


Figure 1.5: A digital signal communication system with additive noise.

and

$$V[X] = \sum_{i=1}^{m} w_i V[X_i] + \sum_{i=1}^{m} w_i \left(\mathbb{E}[X_i] - \mathbb{E}[X]\right)^2,$$

respectively. A mixture distribution can also be defined for countably and uncountably infinite numbers of components. Such distributions, however, are rare in practice.

Example 7: Signal communications. Consider transmission of a single binary digital signal (bit) over a noisy communication channel shown in Figure 1.5. The magnitude of the signal X emitted by the source is equally likely to be 0 or 1 Volt. The signal is sent over a transmission line (e.g., radio communication, optical fiber, magnetic tape) in which a zero-mean normally distributed noise component Y is added to X. Derive the probability distribution of the signal $Z = X + Y$ that enters the receiver.

We will consider a slightly more general situation where X : Bernoulli(α) and Y : Gaussian(μ, σ^2). To find $p(z)$ we will use characteristic functions of random variables X, Y and Z, written as $\varphi_X(t) = \mathbb{E}[e^{itX}]$, $\varphi_Y(t) = \mathbb{E}[e^{itY}]$ and $\varphi_Z(t) = \mathbb{E}[e^{itZ}]$. Without derivation we write

$$\varphi_X(t) = 1 - \alpha + \alpha e^{it}$$
$$\varphi_Y(t) = e^{it\mu - \frac{\sigma^2 t^2}{2}}$$

and subsequently

$$\begin{aligned}
\varphi_Z(t) &= \varphi_{X+Y}(t) \\
&= \varphi_X(t) \cdot \varphi_Y(t) \\
&= \left(1 - \alpha + \alpha e^{it}\right) \cdot e^{it\mu - \frac{\sigma^2 t^2}{2}} \\
&= \alpha e^{it(\mu+1) - \frac{\sigma^2 t^2}{2}} + (1-\alpha) e^{it\mu - \frac{\sigma^2 t^2}{2}}.
\end{aligned}$$

By performing integration on $\varphi_Z(t)$ we can easily verify that

$$p(z) = \alpha \cdot \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(z-\mu-1)^2} + (1-\alpha) \cdot \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(z-\mu)^2},$$

which is a mixture of two normal distributions $\mathcal{N}(\mu+1, \sigma^2)$ and $\mathcal{N}(\mu, \sigma^2)$ with coefficients $w_1 = \alpha$ and $w_2 = 1-\alpha$, respectively. Observe that a convex combination of random variables $Z = w_1 X + w_2 Y$ does not imply $p_Z(x) = w_1 p_X(x) + w_2 p_Y(x)$.

□

1.2 [Advanced] Graphical representation of probability distributions

We saw earlier that a joint probability distribution can be *factorized* using the chain rule from Equation (1.3). Such factorizations can be visualized using a directed graph representation, where nodes represent random variables and edges depict dependence. For example,

$$p(x, y, z) = p(x)p(y|x)p(z|x, y)$$

is shown in Figure 1.6A. Graphical representations of probability distributions using directed acyclic graphs, together with conditional probability distributions, are called *Bayesian networks* or *belief networks*. They facilitate interpretation as well as effective statistical inference.

Visualizing relationships between variables becomes particularly convenient when we want to understand and analyze conditional independence properties of variables. Figure 1.6B shows the the same factorization of $p(x, y, z)$ where variable Z is independent of X given Y. To carefully determine conditional independence and dependence properties, however, one usually uses the *d-separation* rules for belief networks. Though often relationships are intuitive, sometimes dependence properties can get more complicated due to multiple relationships between nodes. For example, in Figure 1.7A, two nodes do not have an edge, but are conditionally dependent through another node. On the other hand, in Figure 1.7B, the absence of an edge does imply conditional independence. We will not further examine d-separation rules at this time; they can easily be found in any standard textbook on graphical models.

Belief networks have a simple, formal definition. Given a set of d random variables $\boldsymbol{X} = (X_1, \ldots, X_d)$, belief networks factorize the joint probability distribution of $\boldsymbol{X}$ as

$$p(\boldsymbol{x}) = \prod_{i=1}^{d} p\left(x_i | \boldsymbol{x}_{\text{Parents}(X_i)}\right),$$

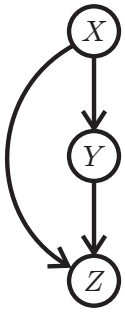
where Parents(X) denotes the immediate ancestors of node X in the graph. In Figure 1.6B, node Y is a parent of Z, but node X is not a parent of Z.

It is important to mention that there are multiple (how many?) ways of factorizing a distribution. For example, by reversing the order of variables $p(x, y, z)$ can be also factorized as

$$p(x, y, z) = p(z)p(y|z)p(x|y, z),$$

which has a different graphical representation and its own conditional probability distributions, yet the same joint probability distribution as the earlier factorization. Selecting a proper factorization and estimating the conditional probability distributions from data will be discussed in detail later.

A. Discrete probability distribution without conditional independences



$P(X=1)$
0.3

X	$P(Y=1\|X)$
0	0.5
1	0.9

X	Y	$P(Z=1\|X,Y)$
0	0	0.3
0	1	0.1
1	0	0.7
1	1	0.4

$$P(X=x, Y=y, Z=z) = P(X=x)P(Y=y|X=x)P(Z=z|X=x, Y=y)$$

B. Discrete probability distribution; Z is conditionally independent of X given Y

$P(X=1)$
0.3

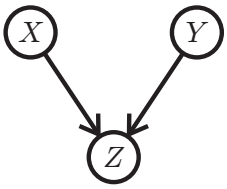
X	$P(Y=1\|X)$
0	0.5
1	0.9

Y	$P(Z=1\|Y)$
0	0.2
1	0.7

$$P(X=x, Y=y, Z=z) = P(X=x)P(Y=y|X=x)P(Z=z|Y=y)$$

Figure 1.6: Bayesian network: graphical representation of two joint probability distributions for three discrete (binary) random variables (X, Y, Z) using directed acyclic graphs. The probability mass function $p(x, y, z)$ is defined over $\{0, 1\}^3$. (A) Full factorization; (B) Factorization that shows and ensures conditional independence between Z and X, given Y. Each node is associated with a conditional probability distribution. In discrete cases, these conditional distributions are referred to as conditional probability tables.

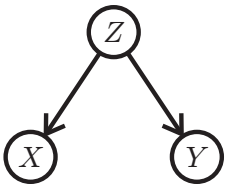
A. X is independent of Y, but not given Z



$$P(X = x \,|\, Y = y) = P(X = x)$$

$$P(X = x \,|\, Y = y, Z = z) \neq P(X = x \,|\, Z = z)$$

B. X and Y are dependent, but conditionally independent given Z



$$P(X = x \,|\, Y = y, Z = z) = P(X = x \,|\, Z = z)$$

$$P(Y = y \,|\, X = x, Z = z) = P(Y = y \,|\, Z = z)$$

Figure 1.7: Two examples of Bayesian networks. (A) A model where the lack of an edge between nodes does not indicate independence. Given information about Z, X and Y are actually dependent; i.e., they are conditionally dependent through Z. (B) A model where the lack of an edge between nodes does indicate independence. Given information about Z, X and Y are conditionally independent. We will see this representation later under Naive Bayes models.

Undirected graphs can also be used to factorize probability distributions. The main idea here is to decompose graphs into maximal cliques $\mathcal{C}$ (the smallest set of cliques that covers the graph) and express the distribution in the following form

$$p(\boldsymbol{x}) = \frac{1}{Z} \prod_{C \in \mathcal{C}} \psi_C(\boldsymbol{x}_C),$$

where each $\psi_C(\boldsymbol{x}_C) \geq 0$ is called the clique potential function and

$$Z = \int_{\boldsymbol{x}} \prod_{C \in \mathcal{C}} \psi_C(\boldsymbol{x}_C) d\boldsymbol{x},$$

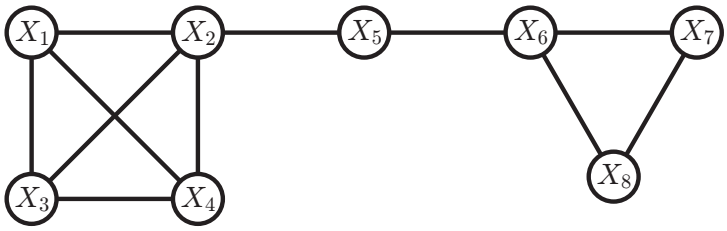
is called the partition function, used strictly for normalization purposes. In contrast to conditional probability distributions in directed acyclic graphs, the clique potentials usually do not have conditional probability interpretations and, thus, normalization is necessary. One example of a maximum clique decomposition is shown in Figure 1.8.

The potential functions are typically taken to be strictly positive, $\psi_C(\boldsymbol{x}_C) > 0$, and expressed as

$$\psi_C(\boldsymbol{x}_C) = \exp\left(-E(\boldsymbol{x}_C)\right),$$

where $E(\boldsymbol{x}_C)$ is a user-specified energy function on the clique of random variables $\boldsymbol{X}_C$. This leads to the probability distribution of the following form

$$p(\boldsymbol{x}) = \frac{1}{Z} \exp\left(\sum_{C \in \mathcal{C}} \log \psi_C(\boldsymbol{x}_C)\right).$$



$$\boldsymbol{X}_{C_1} = \{X_1, X_2, X_3, X_4\} \qquad \boldsymbol{X}_{C_3} = \{X_5, X_6\}$$
$$\boldsymbol{X}_{C_2} = \{X_2, X_5\} \qquad \boldsymbol{X}_{C_4} = \{X_6, X_7, X_8\}$$

Figure 1.8: Markov network: graphical representation of a probability distribution using maximum clique decomposition. Shown is a set of eight random variables with their interdependency structure and maximum clique decomposition (a clique is fully connected subgraph of a given graph). A decomposition into maximum cliques covers all vertices and edges in a graph with the minimum number of cliques. Here, the set of variables is decomposed into four maximal cliques $\mathcal{C} = \{C_1, C_2, C_3, C_4\}$.

As formulated, this probability distribution is called the Boltzmann distribution or the Gibbs distribution.

The energy function $E(\boldsymbol{x})$ must be lower for values of $\boldsymbol{x}$ that are more likely. It also may involve parameters that are then estimated from the available training data. Of course, in a prediction problem, an undirected graph must be created to also involve the target variables, which were here considered to be a subset of $\boldsymbol{X}$.

Consider now any probability distribution over all possible configurations of the random vector $\boldsymbol{X}$ with its underlying graphical representation. If the following property

$$p\left(x_i|\boldsymbol{x}_{-X_i}\right) = p\left(x_i|\boldsymbol{x}_{N(X_i)}\right) \tag{1.7}$$

is satisfied, the probability distribution is referred to as *Markov network* or a *Markov random field*. In the equation above

$$\boldsymbol{X}_{-X_i} = (X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_d)$$

and $N(X)$ is a set of random variables neighboring X in the graph; i.e., there exists an edge between X and every node in $N(X)$. The set of random variables in $N(X)$ is also called the Markov blanket of X.

It can be shown that every Gibbs distribution satisfies the property from Equation (1.7) and, conversely, that for every probability distribution for which Equation (1.7) holds can be represented as a Gibbs distribution with some choice of parameters. This equivalence of Gibbs distributions and Markov networks was established by the Hammersley-Clifford theorem.

Chapter 2

Basic Principles of Parameter Estimation

In probabilistic modeling, we are typically presented with a set of observations and the objective is to find a model, or function, $\hat{f}$ that shows good agreement with the data and respects certain additional requirements. We shall roughly categorize these requirements into three groups: (*i*) the ability to generalize well, (*ii*) the ability to incorporate prior knowledge and assumptions into modeling, and (*iii*) scalability. First, the model should be able to stand the test of time; that is, its performance on the previously unseen data should not deteriorate once this new data is presented. Models with such performance are said to generalize well. Second, $\hat{f}$ must be able to incorporate information about the model space $\mathcal{F}$ from which it is selected and the process of selecting a model should be able to accept training "advice" from an analyst. Finally, when large amounts of data are available, learning algorithms must be able to provide solutions in reasonable time given the resources such as memory or CPU power. In summary, the choice of a model ultimately depends on the observations at hand, our experience with modeling real-life phenomena, and the ability of algorithms to find good solutions given limited resources.

An easy way to think about finding the "best" model is through learning parameters of a distribution. Suppose we are given a set of observations $\mathcal{D} = \{x_i\}_{i=1}^n$, where $x_i \in \mathbb{R}$ and have knowledge that $\mathcal{F}$ is a family of all univariate Gaussian distributions; e.g., $\mathcal{F} = \text{Gaussian}(\mu, \sigma^2)$, with $\mu \in \mathbb{R}$ and $\sigma \in \mathbb{R}^+$. In this case, the problem of finding the best model (by which we mean function) can be seen as finding the best parameters μ^* and σ^*; i.e., the problem can be seen as *parameter estimation*. We call this process estimation because the typical assumption is that the data was generated by an unknown model from $\mathcal{F}$ whose parameters we are trying to recover from data.

We will formalize parameter estimation using probabilistic techniques and will subsequently find solutions through optimization, occasionally with constrains in the parameter space. The main assumption throughout this part will be that the set of observations $\mathcal{D}$ was generated (or collected) independently and according to the same distribution $p(x)$. The statistical framework for model inference is shown in Figure 2.1.

2.1 Maximum a posteriori and maximum likelihood estimation

The idea behind *maximum a posteriori* (MAP) estimation is to find the most probable model for the observed data. Given the data set $\mathcal{D}$, we formalize the MAP solution as

$$f_{\text{MAP}} = \arg\max_{f \in \mathcal{F}} \{p(f|\mathcal{D})\},$$

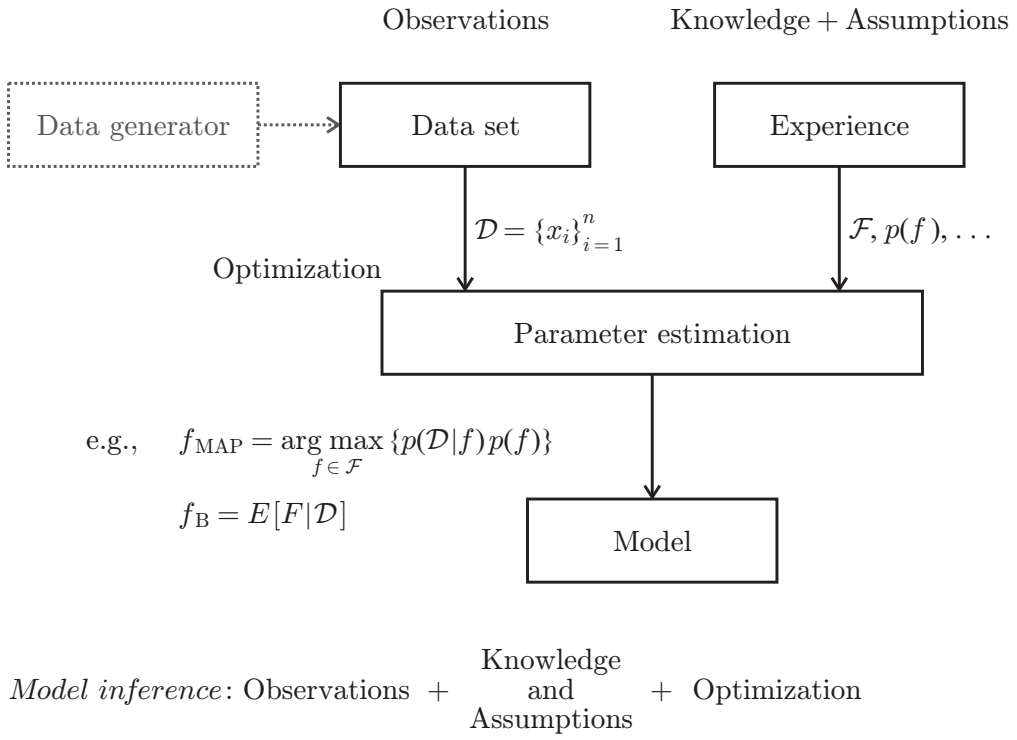


Figure 2.1: Statistical framework for model inference. The estimates of the parameters are made using a set of observations $\mathcal{D}$ as well as experience in the form of model space $\mathcal{F}$, prior distribution $p(f)$, or specific starting solutions in the optimization step.

where $p(f|\mathcal{D})$ is called the *posterior distribution* of the model given the data. In discrete model spaces, $p(f|\mathcal{D})$ is the probability mass function and the MAP estimate is exactly the most probable model. Its counterpart in continuous spaces is the model with the largest value of the posterior density function. Note that we use words *model*, which is a function, and its *parameters*, which are the coefficients of that function, somewhat interchangeably. However, we should keep in mind the difference, even if only for pedantic reasons.

To calculate the posterior distribution we start by applying the Bayes rule as

$$p(f|\mathcal{D}) = \frac{p(\mathcal{D}|f) \cdot p(f)}{p(\mathcal{D})}, \tag{2.1}$$

where $p(\mathcal{D}|f)$ is called the *likelihood* function, $p(f)$ is the *prior* distribution of the model, and $p(\mathcal{D})$ is the *marginal* distribution of the data. Notice that we use $\mathcal{D}$ for the observed data set, but that we usually think of it as a realization of a multidimensional random variable D drawn according to some distribution $p(\mathcal{D})$. Using the formula of total probability, we can express $p(\mathcal{D})$ as

$$p(\mathcal{D}) = \begin{cases} \sum_{f \in \mathcal{F}} p(\mathcal{D}|f)p(f) & f : \text{discrete} \\ \\ \int_{\mathcal{F}} p(\mathcal{D}|f)p(f)df & f : \text{continuous} \end{cases}$$

Therefore, the posterior distribution can be fully described using the likelihood and the prior. The field of research and practice involving ways to determine this distribution and

optimal models is referred to as *inferential statistics*. The posterior distribution is sometimes referred to as inverse probability.

Finding f_{MAP} can be greatly simplified because $p(\mathcal{D})$ in the denominator does not affect the solution. We shall re-write Equation (2.1) as

$$\begin{aligned} p(f|\mathcal{D}) &= \frac{p(\mathcal{D}|f) \cdot p(f)}{p(\mathcal{D})} \\ &\propto p(\mathcal{D}|f) \cdot p(f), \end{aligned}$$

where $\propto$ is the proportionality symbol. Thus, we can find the MAP solution by solving the following optimization problem

$$f_{\text{MAP}} = \arg\max_{f \in \mathcal{F}} \{p(\mathcal{D}|f)p(f)\}.$$

In some situations we may not have a reason to prefer one model over another and can think of $p(f)$ as a constant over the model space $\mathcal{F}$. Then, maximum a posteriori estimation reduces to the maximization of the likelihood function; i.e.,

$$f_{\text{ML}} = \arg\max_{f \in \mathcal{F}} \{p(\mathcal{D}|f)\}.$$

We will refer to this solution as the *maximum likelihood* solution. Formally speaking, the assumption that $p(f)$ is constant is problematic because a uniform distribution cannot be always defined (say, over $\mathbb{R}$), though there are some solutions to this issue using improper priors. Nonetheless, it may be useful to think of the maximum likelihood approach as a separate technique, rather than a special case of MAP estimation, but keep this connection in mind.

Observe that MAP and ML approaches report solutions corresponding to the mode of the posterior distribution and the likelihood function, respectively. We shall later contrast this estimation technique with the view of the Bayesian statistics in which the goal is to minimize the posterior risk. Such estimation typically results in calculating conditional expectations, which can be complex integration problems. From a different point of view, MAP and ML estimates are called *point estimates*, as opposed to estimates that report confidence intervals for a particular group of parameters.

Example 8: Suppose data set $\mathcal{D} = \{2, 5, 9, 5, 4, 8\}$ is an i.i.d. sample from a Poisson distribution with a fixed but unknown parameter λ_0. Find the maximum likelihood estimate of λ_0.

The probability density function of a Poisson distribution is expressed as $p(x|\lambda) = \lambda^x e^{-\lambda}/x!$, with some parameter $\lambda \in \mathbb{R}^+$. We will estimate this parameter as

$$\lambda_{\text{ML}} = \arg\max_{\lambda \in (0,\infty)} \{p(\mathcal{D}|\lambda)\}. \tag{2.2}$$

We can write the likelihood function as

$$\begin{aligned} p(\mathcal{D}|\lambda) &= p(\{x_i\}_{i=1}^n |\lambda) \\ &= \prod_{i=1}^n p(x_i|\lambda) \\ &= \frac{\lambda^{\sum_{i=1}^n x_i} \cdot e^{-n\lambda}}{\prod_{i=1}^n x_i!}. \end{aligned}$$

To find λ that maximizes the likelihood, we will first take a logarithm (a monotonic function) to simplify the calculation, then find its first derivative with respect to λ, and finally equate it with zero to find the maximum. Specifically, we express the log-likelihood $ll(D, \lambda) = \ln p(\mathcal{D}|\lambda)$ as

$$ll(\mathcal{D}, \lambda) = \ln \lambda \sum_{i=1}^{n} x_i - n\lambda - \sum_{i=1}^{n} \ln (x_i!)$$

and proceed with the first derivative as

$$\begin{aligned} \frac{\partial ll(\mathcal{D}, \lambda)}{\partial \lambda} &= \frac{1}{\lambda} \sum_{i=1}^{n} x_i - n \\ &= 0. \end{aligned}$$

By substituting $n = 6$ and values from $\mathcal{D}$, we can compute the solution as

$$\begin{aligned} \lambda_{\text{ML}} &= \frac{1}{n} \sum_{i=1}^{n} x_i \\ &= 5.5, \end{aligned}$$

which is simply a sample mean. The second derivative of the likelihood function is always negative because λ must be positive; thus, the previous expression indeed maximizes the likelihood. Note that to properly maximize this loss, we also need to ensure the constraint $\lambda \in (0, \infty)$ is enforced. Because the solution above is in the constraint set, we know we have the correct solution to Equation (2.2); however, in other situations, we will have to explicitly enforce constraints in the optimization, as we will discuss later.

□

Example 9: Let $\mathcal{D} = \{2, 5, 9, 5, 4, 8\}$ again be an i.i.d. sample from Poisson(λ_0), but now we are also given additional information. Suppose the prior knowledge about λ_0 can be expressed using a gamma distribution $\Gamma(x|k, \theta)$ with parameters $k = 3$ and $\theta = 1$. Find the maximum a posteriori estimate of λ_0.

First, we write the probability density function of the gamma family as

$$\Gamma(x|k, \theta) = \frac{x^{k-1} e^{-\frac{x}{\theta}}}{\theta^k \Gamma(k)},$$

where $x > 0$, $k > 0$, and $\theta > 0$. $\Gamma(k)$ is the gamma function that generalizes the factorial function; when k is an integer, we have $\Gamma(k) = (k-1)!$. The MAP estimate of the parameters can be found as

$$\lambda_{\text{MAP}} = \arg\max_{\lambda \in (0,\infty)} \{p(\mathcal{D}|\lambda) p(\lambda)\}.$$

As before, we can write the likelihood function as

$$p(\mathcal{D}|\lambda) = \frac{\lambda^{\sum_{i=1}^{n} x_i} \cdot e^{-n\lambda}}{\prod_{i=1}^{n} x_i!}$$

and the prior distribution as

$$p(\lambda) = \frac{\lambda^{k-1} e^{-\frac{\lambda}{\theta}}}{\theta^k \Gamma(k)}.$$

Now, we can maximize the logarithm of the posterior distribution $p(\lambda|\mathcal{D})$ using

$$\begin{aligned}\ln p(\lambda|\mathcal{D}) &\propto \ln p(\mathcal{D}|\lambda) + \ln p(\lambda) \\ &= \ln \lambda(k - 1 + \sum_{i=1}^{n} x_i) - \lambda(n + \frac{1}{\theta}) - \sum_{i=1}^{n} \ln x_i! - k \ln \theta - \ln \Gamma(k)\end{aligned}$$

to obtain

$$\begin{aligned}\lambda_{\text{MAP}} &= \frac{k - 1 + \sum_{i=1}^{n} x_i}{n + \frac{1}{\theta}} \\ &= 5\end{aligned}$$

after incorporating all data.

A quick look at λ_{MAP} and λ_{ML} suggests that as n grows, both numerators and denominators in the expressions above become increasingly more similar. In fact, it is a well-known result that, in the limit of infinite samples, both the MAP and ML converge to the same model, f, as long as the prior does not have zero probability on f. This result shows that the MAP estimate approaches the ML solution for large data sets. In other words, large data diminishes the importance of prior knowledge. This is an important conclusion because it simplifies mathematical apparatus necessary for practical inference.

To get some intuition for this result, we will show that the MAP and ML estimates converge to the same solution for the above example with a Poisson distribution. Let $s_n = \sum_{i=1}^{n} x_i$, which is a sample from the random variable $S_n = \sum_{i=1}^{n} X_i$. If $\lim_{n\to\infty} s_n/n^2 = 0$ (i.e., s_n does not grow faster than n^2), then

$$\begin{aligned}|\lambda_{\text{MAP}} - \lambda_{\text{ML}}| &= \left| \frac{k - 1 + s_n}{n + 1/\theta} - \frac{s_n}{n} \right| \\ &= \left| \frac{k - 1}{n + 1/\theta} - \frac{s_n}{n(n + 1/\theta)} \right| \\ &\leq \frac{|k - 1|}{n + 1/\theta} + \frac{s_n}{n(n + 1/\theta)} \qquad \xrightarrow[n\to\infty]{} 0\end{aligned}$$

Note that if $\lim_{n\to\infty} s_n/n^2 \neq 0$, then both estimators go to ∞; however, such a sequence of values has an essentially zero probability of occurring. Consistency theorems for ML and MAP estimation state that convergence to the true parameters occurs "almost surely" or "with probability 1" to indicate that these unbounded sequences constitute a set of measure-zero, under certain reasonable conditions (for more, see [15, Theorem 9.13]).

□

Example 10: Let $\mathcal{D} = \{x_i\}_{i=1}^{n}$ be an i.i.d. sample from a univariate Gaussian distribution. Find the maximum likelihood estimates of the parameters.

We start by forming the log-likelihood function

$$\begin{aligned}\ln p(\mathcal{D}|\mu,\sigma) &= \ln \prod_{i=1}^{n} p(x_i|\mu,\sigma) \\ &= n \ln \frac{1}{\sqrt{2\pi}} + n \ln \frac{1}{\sigma} - \frac{\sum_{i=1}^{n} (x_i - \mu)^2}{2\sigma^2}.\end{aligned}$$

We now compute the partial derivatives of the log-likelihood with respect to all parameters as

$$\frac{\partial}{\partial \mu} \ln p(\mathcal{D}|\mu,\sigma) = \frac{\sum_{i=1}^{n} (x_i - \mu)}{\sigma^2}$$

and

$$\frac{\partial}{\partial \sigma} \ln p(\mathcal{D}|\mu,\sigma) = -\frac{n}{\sigma} + \frac{\sum_{i=1}^{n} (x_i - \mu)^2}{\sigma^3}.$$

From here, we can proceed to derive that

$$\mu_{\text{ML}} = \frac{1}{n} \sum_{i=1}^{n} x_i$$

and

$$\sigma^2_{\text{ML}} = \frac{1}{n} \sum_{i=1}^{n} (x_i - \mu_{\text{ML}})^2 .$$

□

2.2 Maximum likelihood for conditional distributions

We can also formulate maximum likelihood problems for conditional distributions. Recall that a conditional distribution has the form $p(y|x)$, for two random variables Y and X, where above we considered the marginal distribution $p(x)$ or $p(y)$. For the distributions above, we asked: what is the distribution over this variable? For a conditional distribution, we are instead asking: given some auxiliary information, now what is the distribution over this variable? When the auxiliary information changes, so will the distribution over the variable. For example, we may want to condition a distribution over sales of a particular product (Y) given the current month (X). We expect the distribution over Y to be different, depending on the month.

Conditional distributions can be from any of the distribution families discussed above, and we can similarly formulate parameter estimation problems. The parameters, however, are usually tied to the given variable X. We provide a simple example to demonstrate this below. Much of the parameter estimation formulations we consider in the remainder of the book will be for conditional distributions, because in machine learning we typically have a large number of auxiliary variables (features) and are trying to predict (or learn the distribution over) targets. In the chapters on regression and classification, we will

demonstrate how many models can be formulated as maximum likelihood for conditional distributions $p(y|\mathbf{x})$.

Example 11: Assume you are given two random variables X and Y and that you believe $p(y|x) = \mathcal{N}(\mu = x, \sigma^2)$ for some unknown σ. Our goal is to estimate this unknown parameter σ. Notice that the distribution over Y varies, depending on which X value is observed or given.

We again start by forming the log-likelihood function, now for pairs of n samples $\mathcal{D} = (x_1, y_1), \ldots, (x_n, y_n)$. We will use the chain rule: $p(x_i, y_i) = p(y_i|x_i)p(x_i)$.

$$\begin{aligned}
\ln p(\mathcal{D}|\sigma) &= \ln \prod_{i=1}^{n} p(x_i, y_i|\sigma) \\
&= \ln \prod_{i=1}^{n} p(y_i|x_i, \sigma)p(x_i) \\
&= n \ln \frac{1}{\sqrt{2\pi}} + n \ln \frac{1}{\sigma} - \frac{\sum_{i=1}^{n} (y_i - x_i)^2}{2\sigma^2} + \sum_{i=1}^{n} \ln p(x_i).
\end{aligned}$$

Notice that the last line uses $\mu = x_i$ for each normal distribution $p(y_i|x_i, \sigma)$. We now compute the partial derivatives of the log-likelihood with respect to the parameter σ

$$\frac{\partial}{\partial \sigma} \ln p(\mathcal{D}|\sigma) = -\frac{n}{\sigma} + \frac{\sum_{i=1}^{n} (y_i - x_i)^2}{\sigma^3}.$$

Notice that $\frac{\partial}{\partial \sigma} \sum_{i=1}^{n} \ln p(x_i) = 0$, because σ does not parameterize $p(x_i)$. Therefore, to obtain the optimal σ, we do not need to know or specify the distribution over the random variable X. By setting the derivative to zero, to obtain a stationary point, we obtain

$$\sigma^2_{\mathrm{ML}} = \frac{1}{n} \sum_{i=1}^{n} (y_i - x_i)^2.$$

□

2.3 [Advanced] The relationship between maximizing likelihood and Kullback-Leibler divergence

We now investigate the relationship between maximum likelihood estimation and Kullback-Leibler divergence. Kullback-Leibler divergence between two probability distributions $p(x)$ and $q(x)$ is defined on $\mathcal{X} = \mathbb{R}$ as

$$D_{\mathrm{KL}}(p||q) = \int_{-\infty}^{\infty} p(x) \log \frac{p(x)}{q(x)} dx.$$

In information theory, Kullback-Leibler divergence has a natural interpretation of the inefficiency of signal compression when the code is constructed using a suboptimal distribution $q(x)$ instead of the correct (but unknown) distribution $p(x)$ according to which the data has been generated. However, more often than not, Kullback-Leibler divergence is simply considered to be a measure of divergence between two probability distributions. Although this

divergence is not a metric (it is not symmetric and does not satisfy the triangle inequality) it has important theoretical properties in that (i) it is always non-negative and (ii) it is equal to zero if and only if $p(x) = q(x)$.

Consider now a divergence between an estimated probability distribution $p(x|\theta)$ and an underlying (true) distribution $p(x|\theta_0)$ according to which the data set $\mathcal{D} = \{x_i\}_{i=1}^n$ was generated. The Kullback-Leibler divergence between $p(x|\theta)$ and $p(x|\theta_0)$ is

$$\begin{aligned} D_{\mathrm{KL}}(p(x|\theta_0)||p(x|\theta)) &= \int_{-\infty}^{\infty} p(x|\theta_0) \log \frac{p(x|\theta_0)}{p(x|\theta)} dx \\ &= \int_{-\infty}^{\infty} p(x|\theta_0) \log \frac{1}{p(x|\theta)} dx - \int_{-\infty}^{\infty} p(x|\theta_0) \log \frac{1}{p(x|\theta_0)} dx. \end{aligned}$$

The second term in the above equation is simply the (differential) entropy of the true distribution and is not influenced by our choice of the model θ. The first term, on the other hand, can be expressed as

$$\int_{-\infty}^{\infty} p(x|\theta_0) \log \frac{1}{p(x|\theta)} dx = -E[\log p(X|\theta)]$$

Therefore, maximizing $E[\log p(X|\theta)]$ minimizes the Kullback-Leibler divergence between $p(x|\theta)$ and $p(x|\theta_0)$. Using the strong law of large numbers, we know that

$$\frac{1}{n} \sum_{i=1}^{n} \log p(x_i|\theta) \quad \overset{a.s.}{\to} \quad E[\log p(X|\theta)]$$

when $n \to \infty$. Thus, when the data set is sufficiently large, maximizing the likelihood function minimizes the Kullback-Leibler divergence and leads to the conclusion that $p(x|\theta_{\mathrm{ML}}) = p(x|\theta_0)$, if the underlying assumptions are satisfied. Under reasonable conditions, we can infer from it that $\theta_{\mathrm{ML}} = \theta_0$. This will hold for families of distributions for which a set of parameters uniquely determines the probability distribution; e.g., it will not generally hold for mixtures of distributions but we will discuss this situation later. This result is only one of the many connections between statistics and information theory.

Chapter 3

Introduction to Prediction Problems

3.1 Problem Statement

We start by defining a data set $\mathcal{D} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), ..., (\mathbf{x}_n, y_n)\}$, where $\mathbf{x}_i \in \mathcal{X}$ is the i-th object and $y_i \in \mathcal{Y}$ is the corresponding target designation. We usually assume that $\mathcal{X} = \mathbb{R}^d$, in which case $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{id})$ is a d-dimensional vector called a *data point* (or *example* or *sample*). Each dimension of $\mathbf{x}_i$ is typically called a *feature* or an *attribute*.

We generally distinguish between two related but different types of prediction problems: classification and regression. Generally speaking, we have a classification problem if $\mathcal{Y}$ is discrete and a regression problem when $\mathcal{Y}$ is continuous. The *classification problem* refers to constructing a function that for a previously unseen data point $\mathbf{x}$ infers (predicts) its class label y. A particular function or algorithm that infers class labels, and is typically optimized to minimize or maximize some objective (or fitness) function, is referred to as a *classifier* or a *classification model*. The cardinality of $\mathcal{Y}$ in classification problems is usually small, e.g. $\mathcal{Y} = \{\text{healthy, disease}\}$. On the other hand, the *regression problem* refers to constructing a model that for a previously unseen data point $\mathbf{x}$ approximates the target value y as closely as possible, where often times $\mathcal{Y} = \mathbb{R}$.

An example of a data set for classification with $n = 3$ data points and $d = 5$ features is shown in Table 3.1. Problems in which $|\mathcal{Y}| = 2$ are referred to as binary classification problems, whereas problems in which $|\mathcal{Y}| > 2$ are referred to as multi-class classification problems. This can be more complex as, for instance, in classification of text documents into categories such as $\{\text{sports, medicine, travel}, \ldots\}$. Here, a single document may be related to more than one value in the set; e.g. an article on sports medicine. To account for this, we can certainly say that $\mathcal{Y} = \mathcal{P}(\{\text{sports, medicine, travel}, \ldots\})$ and treat the problem as multi-class classification, albeit with a very large output space. However, it is often easier to think that more than one value of the output space can be associated with any particular input. We refer to this learning task as multi-label classification and set $\mathcal{Y} = \{\text{sports, medicine, travel}, \ldots\}$. Finally, $\mathcal{Y}$ can be a set of structured outputs, e.g. strings, trees, or graphs. This classification scenario is usually referred to as structured-output learning. The cardinality of the output space in structured-output learning problems is often very high. An example of a regression problem is shown in Table 3.2.

In both prediction scenarios, we assume that the features are easy to collect for each object (e.g. by measuring the height of a person or the square footage of a house), while the target variable is difficult to observe or expensive to collect. Such situations usually benefit from the construction of a computational model that predicts targets from a set of input values. The model is trained using a set of input objects for which target values have already been collected.

Observe that there does not exist a strict distinction between classification and regres-

	wt [kg]	ht [m]	T [°C]	sbp [mmHg]	dbp [mmHg]	y
$\mathbf{x}_1$	91	1.85	36.6	121	75	-1
$\mathbf{x}_2$	75	1.80	37.4	128	85	$+1$
$\mathbf{x}_3$	54	1.56	36.6	110	62	-1

Table 3.1: An example of a binary classification problem: prediction of a disease state for a patient. Here, features indicate weight (wt), height (ht), temperature (T), systolic blood pressure (sbp), and diastolic blood pressure (dbp). The class labels indicate presence of a particular disease, e.g. diabetes. This data set contains one positive data point ($\mathbf{x}_2$) and two negative data points ($\mathbf{x}_1$, $\mathbf{x}_3$). The class label shows a disease state, i.e. $y_i = +1$ indicates the presence while $y_i = -1$ indicates absence of disease.

	size [sqft]	age [yr]	dist [mi]	inc [$]	dens [ppl/mi^2]	y
$\mathbf{x}_1$	1250	5	2.85	56,650	12.5	2.35
$\mathbf{x}_2$	3200	9	8.21	245,800	3.1	3.95
$\mathbf{x}_3$	825	12	0.34	61,050	112.5	5.10

Table 3.2: An example of a regression problem: prediction of the price of a house in a particular region. Here, features indicate the size of the house (size) in square feet, the age of the house (age) in years, the distance from the city center (dist) in miles, the average income in a one square mile radius (inc), and the population density in the same area (dens). The target indicates the price a house is sold at, e.g. in hundreds of thousands of dollars.

sion. For example, if the output space is $\mathcal{Y} = \{0, 1, 2\}$, we need not treat this problem as classification. This is because there exists a relationship of order among elements of $\mathcal{Y}$ that can simplify model development. For example, we can take $\mathcal{Y} = [0, 2]$ and simply develop a regression model from which we can recover the original discrete values by rounding the raw prediction outputs. The selection of a particular way of modeling depends on the analyst and their knowledge of the domain as well as technical aspects of learning.

3.2 Formal notation for prediction

In the machine learning literature we use d-tuples $\mathbf{x} = (x_1, x_2, \ldots, x_d)$ to denote data points. However, often times we can benefit from the algebraic notation, where each data point $\mathbf{x}$ is a column vector in the d-dimensional Euclidean space: $\mathbf{x} = [x_1\ x_2\ \ldots\ x_d]^\top \in \mathbb{R}^d$, where $\top$ is the transpose operator. Here, a linear combination of features and some set of coefficients $\mathbf{w} = [w_1\ w_2\ \ldots\ w_d]^\top \in \mathbb{R}^d$

$$\sum_{i=1}^{d} w_i x_i = w_1 x_1 + w_2 x_2 + \ldots + w_d x_d$$

can be expressed using an inner (dot) product of column vectors $\mathbf{w}^\top \mathbf{x}$. A linear combination $\mathbf{w}^\top \mathbf{x}$ results in a single number. Another useful notation for such linear combinations will be $\langle \mathbf{w}, \mathbf{x} \rangle$.

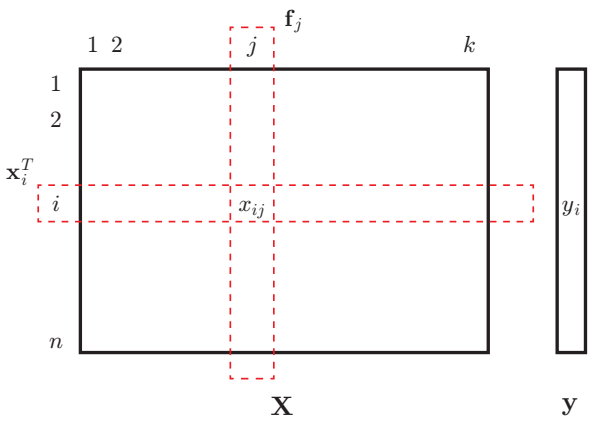


Figure 3.1: Data set representation and notation. $\mathbf{x}$ *is an* n*-by-*d *matrix representing features and data points, whereas* y *is an* n*-by-*1 *vector of targets.*

We will also use an n-by-d matrix $\mathbf{x} = (\mathbf{x}_1^\top, \mathbf{x}_2^\top, \ldots, \mathbf{x}_n^\top)$ to represent the entire set of data points and $\mathbf{y}$ to represent a column vector of targets. For example, the i-th row of $\mathbf{x}$ represents data point $\mathbf{x}_i^\top$. Finally, the j-th column of $\mathbf{x}$, denoted as $\mathbf{f}_j$, is an n-by-1 vector which contains the values of feature j for all data points. The notation is further presented in Figure 3.1.

3.3 Optimal classification and regression models

Our goal now is to establish the performance criteria that will be used to evaluate predictors $f : \mathcal{X} \to \mathcal{Y}$ and subsequently define optimal classification and regression models. We start with classification and consider a situation where the joint probability distribution $p(\mathbf{x}, y)$ is either known or can be learned from data. Also, we will consider that we are given a cost function $c : \mathcal{Y} \times \mathcal{Y} \to [0, \infty)$, where for each prediction $\hat{y}$ and true target value y the classification cost can be expressed as a constant $c(\hat{y}, y)$, regardless of the input $\mathbf{x} \in \mathcal{X}$ given to the classifier. This cost function can simply be stored as a $|\mathcal{Y}| \times |\mathcal{Y}|$ cost matrix.

The criterion for optimality of a classifier will be probabilistic. In particular, we are interested in minimizing the expected cost

$$\begin{aligned}\mathbb{E}[C] &= \int_{\mathcal{X}} \sum_{y} c(\hat{y}, y) p(\mathbf{x}, y) d\mathbf{x} \\ &= \int_{\mathcal{X}} p(\mathbf{x}) \sum_{y} c(\hat{y}, y) p(y|\mathbf{x}) d\mathbf{x},\end{aligned}$$

where the integration is over the entire input space $\mathcal{X} = \mathbb{R}^d$. From this equation, we can see that the optimal classifier can be expressed as

$$f_{\mathrm{BR}}(\mathbf{x}) = \arg\min_{\hat{y} \in \mathcal{Y}} \left\{ \sum_{y} c(\hat{y}, y) p(y|\mathbf{x}) \right\},$$

for any $\mathbf{x} \in \mathcal{X}$. We will refer to this classifier as the *Bayes risk classifier*. One example where the Bayes risk classifier can be useful is the medical domain. Suppose our goal is to decide

whether a patient with a particular set of symptoms ($\mathbf{x}$) should be sent for an additional lab test ($y = 1$ if yes and $y = -1$ if not), with cost c_{lab}, in order to improve diagnosis. However, if we do not perform a lab test and the patient is later found to have needed the test for proper treatment, we may incur a significant penalty, say c_{lawsuit}. If $c_{\text{lawsuit}} \gg c_{\text{lab}}$, as it is expected to be, then the classifier needs to appropriately adjust its outputs to account for the cost disparity in different forms of incorrect prediction.

In many practical situations, however, it may not be possible to define a meaningful cost matrix and, thus, a reasonable criterion would be to minimize the probability of a classifier's error $P(f(\mathbf{x}) \neq y)$. This corresponds to the situation where the cost function is defined as

$$c(\hat{y}, y) = \begin{cases} 0 & \text{when } y = \hat{y} \\ \\ 1 & \text{when } y \neq \hat{y} \end{cases}$$

After plugging these values in the definition for $f_{\text{BR}}(\mathbf{x})$, the Bayes risk classifier simply becomes the maximum a posteriori (MAP) classifier. That is,

$$f_{\text{MAP}}(\mathbf{x}) = \arg\max_{y \in \mathcal{Y}} \{p(y|\mathbf{x})\}.$$

Therefore, if $p(y|\mathbf{x})$ is known or can be accurately learned, we are fully equipped to make the prediction that minimizes the total cost. In other words, we have converted the problem of minimizing the expected classification cost or probability of error, into the problem of learning functions, more specifically learning probability distributions.

The analysis for regression is a natural extension of that for classification. Here too, we are interested in minimizing the expected cost of prediction of the true target y when a predictor $f(\mathbf{x})$ is used. The expected cost can be expressed as

$$\mathbb{E}[C] = \int_{\mathcal{X}} \int_{\mathcal{Y}} c(f(\mathbf{x}), y) p(\mathbf{x}, y) dy d\mathbf{x},$$

where $c : \mathbb{R} \times \mathbb{R} \to [0, \infty)$ is again some cost function between the predicted value $f(\mathbf{x})$ and the true value y. For simplicity, we will consider

$$c(f(\mathbf{x}), y) = (f(\mathbf{x}) - y)^2,$$

which results in

$$\begin{aligned} \mathbb{E}[C] &= \int_{\mathcal{X}} \int_{\mathcal{Y}} (f(\mathbf{x}) - y)^2 p(\mathbf{x}, y) dy d\mathbf{x} \\ &= \int_{\mathcal{X}} p(\mathbf{x}) \underbrace{\int_{\mathcal{Y}} (f(\mathbf{x}) - y)^2 p(y|\mathbf{x}) dy}_{g(f(\mathbf{x}))} d\mathbf{x}. \end{aligned}$$

Assuming $f(\mathbf{x})$ is flexible enough to be separately optimized for each unit volume $d\mathbf{x}$, we see that minimizing $\mathbb{E}[C]$ leads us to the problem of minimizing

$$g(u) = \int_{\mathcal{Y}} (u - y)^2 p(y|\mathbf{x}) dy,$$

where we used a substitution $u = f(\mathbf{x})$. We can now differentiate g with respect to u as

$$\begin{aligned}\frac{\partial g(u)}{\partial u} &= 2\int_{\mathcal{Y}} (u - y)p(y|\mathbf{x})dy = 0 \\ \implies u\underbrace{\int_{\mathcal{Y}} p(y|\mathbf{x})dy}_{=1} &= \int_{\mathcal{Y}} yp(y|\mathbf{x})dy\end{aligned}$$

which results in the optimal solution

$$\begin{aligned}f^*(\mathbf{x}) &= \int_{\mathcal{Y}} yp(y|\mathbf{x})dy \\ &= \mathbb{E}[Y|\mathbf{x}].\end{aligned}$$

Therefore, the optimal regression model in the sense of minimizing the square error between the prediction and the true target is the conditional expectation $\mathbb{E}[Y|\mathbf{x}]$. It may appear that in the above equations, setting $f(\mathbf{x}) = y$ would always lead to $\mathbb{E}[C] = 0$. Unfortunately, this would be an invalid operation because for a single input $\mathbf{x}$ there may be multiple possible outputs y and they can certainly appear in the same data set. To be a well-defined function, $f(\mathbf{x})$ must always have the same output for the same input. $\mathbb{E}[C] = 0$ can only be achieved if $p(y|\mathbf{x})$ is a delta function for every $\mathbf{x}$.

Having found the optimal regression model, we can now write the expected cost in the cases of both optimal and suboptimal models $f(\mathbf{x})$. That is, we are interested in expressing $\mathbb{E}[C]$ when

1. $f(\mathbf{x}) = \mathbb{E}[Y|\mathbf{x}]$
2. $f(\mathbf{x}) \neq \mathbb{E}[Y|\mathbf{x}]$.

We have already found $\mathbb{E}[C]$ when $f(\mathbf{x}) = \mathbb{E}[Y|\mathbf{x}]$. The expected cost can be simply expressed as

$$\mathbb{E}[C] = \int_{\mathcal{X}}\int_{\mathcal{Y}} (\mathbb{E}[Y|\mathbf{x}] - y)^2 p(\mathbf{x}, y)dyd\mathbf{x},$$

which corresponds to the (weighted) squared error between the optimal prediction and the target everywhere in the feature space. This is the best scenario in regression; we cannot achieve a lower cost on average for this squared cost.

The next situation is when $f(\mathbf{x}) \neq \mathbb{E}[Y|\mathbf{x}]$. Here, we will proceed by decomposing the squared error as

$$\begin{aligned}(f(\mathbf{x}) - y)^2 &= (f(\mathbf{x}) - \mathbb{E}[Y|\mathbf{x}] + \mathbb{E}[Y|\mathbf{x}] - y)^2 \\ &= (f(\mathbf{x}) - \mathbb{E}[Y|\mathbf{x}])^2 + 2\underbrace{(f(\mathbf{x}) - \mathbb{E}[Y|\mathbf{x}])(\mathbb{E}[Y|\mathbf{x}] - y)}_{g(\mathbf{x},y)} + (\mathbb{E}[Y|\mathbf{x}] - y)^2\end{aligned}$$

We will now take a more detailed look at $g(\mathbf{x}, y)$ when placed under the expectation over

$p(\mathbf{x}, y)$

$$\begin{aligned}
\mathbb{E}[g(\boldsymbol{X}, y)] &= \int_{\mathcal{X}} \int_{\mathcal{Y}} (f(\mathbf{x}) - \mathbb{E}[Y|\mathbf{x}])(\mathbb{E}[Y|\mathbf{x}] - y) p(\mathbf{x}, y) dy d\mathbf{x} \\
&= \int_{\mathcal{X}} \int_{\mathcal{Y}} f(\mathbf{x}) \mathbb{E}[Y|\mathbf{x}] p(\mathbf{x}, y) dy d\mathbf{x} - \int_{\mathcal{X}} \int_{\mathcal{Y}} f(\mathbf{x}) y p(\mathbf{x}, y) dy d\mathbf{x} \\
&\quad + \int_{\mathcal{X}} \int_{\mathcal{Y}} \mathbb{E}[Y|\mathbf{x}] y p(\mathbf{x}, y) dy d\mathbf{x} - \int_{\mathcal{X}} \int_{\mathcal{Y}} \mathbb{E}[Y|\mathbf{x}] \mathbb{E}[Y|\mathbf{x}] p(\mathbf{x}, y) dy d\mathbf{x} \\
&= \int_{\mathcal{X}} f(\mathbf{x}) \mathbb{E}[Y|\mathbf{x}] p(\mathbf{x}) d\mathbf{x} - \int_{\mathcal{X}} f(\mathbf{x}) p(\mathbf{x}) \int_{\mathcal{Y}} y p(y|\mathbf{x}) dy d\mathbf{x} \\
&\quad \int_{\mathcal{X}} \mathbb{E}[Y|\mathbf{x}] \mathbb{E}[Y|\mathbf{x}] p(\mathbf{x}) d\mathbf{x} - \int_{\mathcal{X}} \mathbb{E}[Y|\mathbf{x}] \mathbb{E}[Y|\mathbf{x}] p(\mathbf{x}) d\mathbf{x} \\
&= 0.
\end{aligned}$$

Therefore, we can now express the expected cost as

$$\begin{aligned}
\mathbb{E}[C] &= \int_{\mathcal{X}} \int_{\mathcal{Y}} (f(\mathbf{x}) - y)^2 p(\mathbf{x}, y) dy d\mathbf{x} \\
&= \int_{\mathcal{X}} (f(\mathbf{x}) - \mathbb{E}[Y|\mathbf{x}])^2 p(\mathbf{x}) d\mathbf{x} + \int_{\mathcal{X}} \int_{\mathcal{Y}} (\mathbb{E}[Y|\mathbf{x}] - y)^2 p(\mathbf{x}, y) dy d\mathbf{x},
\end{aligned}$$

where the first term is the "distance" between the trained model $f(\mathbf{x})$ and the optimal model $\mathbb{E}[Y|\mathbf{x}]$ and the second term is the "distance" between the optimal model $\mathbb{E}[Y|\mathbf{x}]$ and the correct target value y. These terms are also often called the *reducible* and *irreducible* errors. If we extend the class of functions f to predict $\mathbb{E}[Y|\mathbf{x}]$, we can reduce the first expected error. However, the second distance is an inherent error, where for any inputs $\mathbf{x}$, there is a distribution over possible values that we can observe. This relates to the problem of partial observability, where there is always some stochasticity due to a lack of information. This irreducible distance could potentially be further reduced by providing more feature information (i.e., extending the information in $\mathbf{x}$). However, for a given dataset, with the given features, this error is irreducible.

To sum up, we argued here that optimal classification and regression models critically depend on knowing or accurately learning the posterior distribution $p(y|\mathbf{x})$. This task can be solved in different ways, but a straightforward approach is to assume a functional form for $p(y|\mathbf{x})$, say $p(y|\mathbf{x}, \boldsymbol{\theta})$, where $\boldsymbol{\theta}$ is a set of weights or parameters that are to be learned from the data. Alternatively, we can learn the class-conditional and prior distributions, $p(\mathbf{x}|y)$ and $p(y)$, respectively. Using

$$\begin{aligned}
p(y|\mathbf{x}) &= \frac{p(\mathbf{x}, y)}{p(\mathbf{x})} \\
&= \frac{p(\mathbf{x}|y)p(y)}{\sum_y p(\mathbf{x}, y)} \\
&= \frac{p(\mathbf{x}|y)p(y)}{\sum_y p(\mathbf{x}|y)p(y)}
\end{aligned}$$

we can see that these two learning approaches are equivalent in theory. The choice depends on our prior knowledge and/or preferences.

Models obtained by directly estimating $p(y|\mathbf{x})$ are called *discriminative models* and models obtained by directly estimating $p(\mathbf{x}|y)$ and $p(y)$ are called *generative models*. Direct estimation of the joint distribution $p(\mathbf{x}, y)$ is relatively rare as it may be more difficult to hypothesize its parametric or non-parametric form from which the parameters are to be found. Finally, in some situations we can train a model without an explicit probabilistic approach in mind. In these cases, we typically aim to show a good performance of an algorithm in practice, say on a large number of data sets, according to a performance measure relevant to the problems at hand.

3.4 [Advanced] Bayes Optimal Models

We saw earlier that optimal prediction models reduce to the learning of the posterior distribution $p(y|\mathbf{x})$ which is then used to minimize the expected cost (risk, loss). However, in practice, the probability distribution $p(y|\mathbf{x})$ must be modeled using a particular functional form and a set of tunable coefficients. When $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{Y} = \{0, 1\}$, one such example is used in logistic regression, where

$$p(1|\mathbf{x}) = \frac{1}{1 + e^{-(w_0 + \sum_{j=1}^{d} w_j x_j)}}$$

and $p(0|\mathbf{x}) = 1 - p(1|\mathbf{x})$. Here $(w_0, w_1, \ldots, w_d) \in \mathbb{R}^{d+1}$ is a set of weights that are to be inferred from a given data set $\mathcal{D}$ and $\mathbf{x} \in \mathbb{R}^d$ is an input data point. A number of other types of functional relationships can be used as well, providing a vast set of possibilities for modeling distributions. We will adjust our notation to more precisely denote the posterior distribution as

$$p(y|\mathbf{x}) = p(y|\mathbf{x}, f),$$

where f is a particular function from some function (hypothesis) space $\mathcal{F}$. We can think of $\mathcal{F}$ as a set of all functions from a specified class, say for all $(w_0, w_1, \ldots, w_d) \in \mathbb{R}^{k+1}$ in the example above, but we can also extend the functional class beyond simple parameter variation to incorporate non-linear decision surfaces.

In a typical learning problem, we are given a data set $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ and are asked to model $p(y|\mathbf{x})$. For this purpose, we will think of $\mathcal{D}$ as a realization of a random variable D and will assume that $\mathcal{D}$ was drawn according to the true underlying distribution $p(\mathbf{x}, y)$. Thus, our task is to express $p(y|\mathbf{x}, \mathcal{D})$. Using the sum and product rules, will rewrite our original task of estimating $p(y|\mathbf{x})$ as

$$\begin{aligned} p(y|\mathbf{x}, \mathcal{D}) &= \int_{\mathcal{F}} p(y|\mathbf{x}, f, \mathcal{D}) p(f|\mathbf{x}, \mathcal{D}) df \\ &= \int_{\mathcal{F}} p(y|\mathbf{x}, f) p(f|\mathbf{x}, \mathcal{D}) df. \end{aligned}$$

Here we used conditional independence between output Y and the data set D once a particular model f was selected based on $\mathcal{D}$; thus $p(y|\mathbf{x}, f, \mathcal{D}) = p(y|\mathbf{x}, f)$. This equation, gives us a sense that the optimal decision can be made through a mixture of distributions $p(y|\mathbf{x}, f)$,

where the weights are given as posterior densities $p(f|\mathbf{x}, \mathcal{D})$. In finite hypothesis spaces $\mathcal{F}$ we have that

$$p(y|\mathbf{x}, \mathcal{D}) = \sum_{f \in \mathcal{F}} p(y|\mathbf{x}, f) p(f|\mathbf{x}, \mathcal{D}),$$

and $p(f|\mathbf{x}, \mathcal{D})$ are posterior probabilities. We may further assume that $p(f|\mathbf{x}, \mathcal{D}) = p(f|\mathcal{D})$, in which case the weights can be precomputed based on the given data set $\mathcal{D}$. This leads to more efficient calculations of the posterior probabilities.

In classification, we can rewrite our original MAP classifier as

$$f_{\text{MAP}}(\mathbf{x}, \mathcal{D}) = \arg\max_{y \in \mathcal{Y}} \left\{ p(y|\mathbf{x}, \mathcal{D}) \right\},$$

which readily leads to the following formulation

$$\begin{aligned} f_{\text{MAP}}(\mathbf{x}, \mathcal{D}) &= \arg\max_{y \in \mathcal{Y}} \left\{ \int_{\mathcal{F}} p(y|\mathbf{x}, f, \mathcal{D}) p(f|\mathcal{D}) df \right\} \\ &= \arg\max_{y \in \mathcal{Y}} \left\{ \int_{\mathcal{F}} p(y|\mathbf{x}, f) p(\mathcal{D}|f) p(f) df \right\}. \end{aligned}$$

It can be shown that no classifier can outperform the *Bayes optimal classifier*. Interestingly, the Bayes optimal model also hints that a better prediction performance can be achieved by combining multiple models and averaging their outputs. This provides theoretical support for ensemble learning and methods such as bagging and boosting.

One problem in Bayes optimal classification is efficient calculation of $f_{\text{MAP}}(\mathbf{x}, \mathcal{D})$, given that the function (hypothesis) space $\mathcal{F}$ is generally uncountable. One approach to this is sampling of functions from $\mathcal{F}$ according to $p(f)$ and then calculating $p(f|\mathcal{D})$ or $p(\mathcal{D}|f)$. This can be computed until $p(y|\mathbf{x}, \mathcal{D})$ converges.

Chapter 4

Linear Regression

Given a data set $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ the objective is to learn the relationship between features and the target. We usually start by hypothesizing the functional form of this relationship. For example,

$$f(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2$$

where $\mathbf{w} = (w_0, w_1, w_2)$ is a set of parameters that need to be determined (learned) and $\mathbf{x} = (x_1, x_2)$. Alternatively, we may hypothesize that $f(\mathbf{x}) = \alpha + \beta x_1 x_2$, where $\boldsymbol{\theta} = (\alpha, \beta)$ is another set of parameters to be learned. In the former case, the target function is modeled as a *linear combination* of features and parameters, i.e.

$$f(\mathbf{x}) = \sum_{j=0}^{d} w_j x_j,$$

where we extended $\mathbf{x}$ to $(x_0 = 1, x_1, x_2, \ldots, x_d)$. Finding the best parameters $\mathbf{w}$ is then referred to as *linear regression problem*, whereas all other types of relationship between the features and the target fall into a category of *non-linear regression*. In either situation, the regression problem can be presented as a probabilistic modeling approach that reduces to parameter estimation; i.e. to an optimization problem with the goal of maximizing or minimizing some performance criterion between target values $\{y_i\}_{i=1}^n$ and predictions $\{f(\mathbf{x}_i)\}_{i=1}^n$. We can think of a particular optimization algorithm as the *learning* or *training algorithm*.

4.1 Maximum likelihood formulation

We now consider a statistical formulation of linear regression. We shall first lay out the assumptions behind this process and subsequently formulate the problem through maximization of the conditional likelihood function. In following section, we will show how to solve the optimization and analyze the solution and its basic statistical properties.

Let us assume that the observed data set $\mathcal{D}$ is a product of a data generating process in which n data points were drawn independently and according to the same distribution $p(\mathbf{x})$. Assume also that the target variable Y has an underlying linear relationship with features $(X_1, X_2, \ldots, X_d)$, modified by some error term ε that follows a zero-mean Gaussian distribution, i.e. $\varepsilon : \mathcal{N}(0, \sigma^2)$. That is, for a given input $\mathbf{x}$, the target y is a realization of a random variable Y defined as

$$Y = \sum_{j=0}^{d} \omega_j X_j + \varepsilon,$$

where $\boldsymbol{\omega} = (\omega_0, \omega_1, \ldots, \omega_d)$ is a set of unknown coefficients we seek to recover through estimation. Generally, the assumption of normality for the error term is reasonable (recall the central limit theorem!), although the independence between ε and $\mathbf{x}$ may not hold in practice. Using a few simple properties of expectations, we can see that Y also follows a Gaussian distribution, i.e. its conditional density is $p(y|\mathbf{x}, \boldsymbol{\omega}) = \mathcal{N}(\boldsymbol{\omega}^\top \mathbf{x}, \sigma^2)$.

In linear regression, we seek to approximate the target as $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$, where weights $\mathbf{w}$ are to be determined. We first write the conditional likelihood function for a single pair $(\mathbf{x}, y)$ as

$$p(y|\mathbf{x}, \mathbf{w}) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\left(y - \sum_{j=0}^{d} w_j x_j\right)^2}{2\sigma^2}}$$

and observe that the only change from the conditional density function of Y is that coefficients $\mathbf{w}$ are used instead of $\boldsymbol{\omega}$. Incorporating the entire data set $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$, we can now write the conditional likelihood function as $p(\mathbf{y}|\mathbf{X}, \mathbf{w})$ and find weights as

$$\mathbf{w}_{\mathrm{ML}} = \arg\max_{\mathbf{w}} \left\{ p(\mathbf{y}|\mathbf{X}, \mathbf{w}) \right\}.$$

Since examples $\mathbf{x}$ are independent and identically distributed (i.i.d.), we have

$$\begin{aligned} p(\mathbf{y}|\mathbf{X}, \mathbf{w}) &= \prod_{i=1}^{n} p(y_i|\mathbf{x}_i, \mathbf{w}) \\ &= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\left(y_i - \sum_{j=0}^{d} w_j x_{ij}\right)^2}{2\sigma^2}}. \end{aligned}$$

For the reasons of mathematical convenience, we will look at the logarithm (monotonic function) of the likelihood function and express the log-likelihood as

$$\ln(p(\mathbf{y}|\mathbf{X}, \mathbf{w})) = -\sum_{i=1}^{n} \log\left(\sqrt{2\pi\sigma^2}\right) - \frac{1}{2\sigma^2} \sum_{i=1}^{n} \left(y_i - \sum_{j=0}^{d} w_j x_{ij} \right)^2.$$

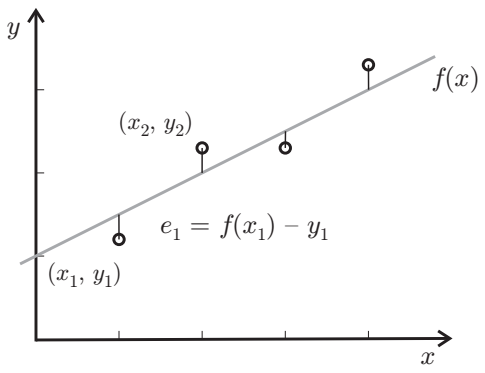


Figure 4.1: An example of a linear regression fitting on data set $\mathcal{D} = \{(1, 1.2), (2, 2.3), (3, 2.3), (4, 3.3)\}$. *The task of the optimization process is to find the best linear function* $f(x) = w_0 + w_1 x$ *so that the sum of squared errors* $e_1^2 + e_2^2 + e_3^2 + e_4^2$ *is minimized.*

Given that the first term on the right-hand hand side is independent of $\mathbf{w}$, maximizing the likelihood function corresponds exactly to minimizing the sum of squared errors

$$\begin{aligned} \text{Err}(\mathbf{w}) &= \sum_{i=1}^{n} \left(f(\mathbf{x}_i) - y_i\right)^2 \qquad \triangleright\, f(\mathbf{x}_i) = \sum_{j=0}^{d} w_j x_{ij} \\ &= \sum_{i=1}^{n} e_i^2. \end{aligned}$$

Geometrically, this error is the square of the Euclidean distance between the vector of predictions $\hat{\mathbf{y}} = (f(\mathbf{x}_1), f(\mathbf{x}_2), \ldots, f(\mathbf{x}_n))$ and the vector of observed target values $\mathbf{y} = (y_1, y_2, \ldots, y_n)$. A simple example illustrating the linear regression problem is shown in Figure 4.1.

To more explicitly see why the maximum likelihood solution corresponds to minimizing $\text{Err}(\mathbf{w})$, notice that maximizing the likelihood is equivalent to maximizing the log-likelihood (because log is monotonic) which is equivalent to minimizing the negative log-likelihood. Therefore, the maximum likelihood $\mathbf{w}_{\text{ML}}$ corresponds to

$$\begin{aligned} \mathbf{w}_{\text{ML}} &= \underset{\mathbf{w}\in\mathbb{R}^d}{\text{argmin}} - \ln(p(\mathbf{y}|\mathbf{X}, \mathbf{w})) \\ &= \underset{\mathbf{w}\in\mathbb{R}^d}{\text{argmin}} \sum_{i=1}^{n} \log\left(\sqrt{2\pi\sigma^2}\right) + \frac{1}{2\sigma^2} \sum_{i=1}^{n} \left(y_i - \sum_{j=0}^{d} w_j x_{ij}\right)^2 \\ &= \underset{\mathbf{w}\in\mathbb{R}^d}{\text{argmin}} \sum_{i=1}^{n} \left(y_i - \sum_{j=0}^{d} w_j x_{ij}\right)^2 \\ &= \underset{\mathbf{w}\in\mathbb{R}^d}{\text{argmin}}\, \text{Err}(\mathbf{w}) \end{aligned}$$

In the next sections, we will discuss how to solve this optimization and the properties of the solution.

Note that we could have simply started with some (expert-defined) error function, as was originally done for OLS and using $\text{Err}(\mathbf{w})$. However, the statistical framework provides insights into the assumptions behind OLS regression. In particular, the assumptions include that the data $\mathcal{D}$ was drawn i.i.d.; there is an underlying linear relationship between features and the target; that the noise (error term) is zero-mean Gaussian and independent of the features; and that there is an absence of noise in the collection of features.

4.2 Ordinary Least-Squares (OLS) Regression

To minimize the sum of squared errors, we shall first re-write $\text{Err}(\mathbf{w})$ as

$$\begin{aligned}\text{Err}(\mathbf{w}) &= \sum_{i=1}^{n} \left(f(\mathbf{x}_i) - y_i\right)^2 \\ &= \sum_{i=1}^{n} \left(\sum_{j=0}^{d} w_j x_{ij} - y_i\right)^2,\end{aligned}$$

where, again, we expanded each data point $\mathbf{x}_i$ by $x_{i0} = 1$ to simplify the expression.

We now calculate the gradient $\nabla\text{Err}(\mathbf{w})$ and the Hessian matrix $H_{\text{Err}(\mathbf{w})}$. Finding weights for which $\nabla\text{Err}(\mathbf{w}) = \mathbf{0}$ will result in an extremum while a positive semi-definite Hessian will ensure that the extremum is a minimum. Now, we set the partial derivatives to 0 and solve the equations for each weight w_j

$$\begin{aligned}\frac{\partial \text{Err}}{\partial w_0} &= 2\sum_{i=1}^{n} \left(\sum_{j=0}^{d} w_j x_{ij} - y_i\right) x_{i0} = 0 \\ \frac{\partial \text{Err}}{\partial w_1} &= 2\sum_{i=1}^{n} \left(\sum_{j=0}^{d} w_j x_{ij} - y_i\right) x_{i1} = 0 \\ &\vdots \\ \frac{\partial \text{Err}}{\partial w_d} &= 2\sum_{i=1}^{n} \left(\sum_{j=0}^{d} w_j x_{ij} - y_i\right) x_{ik} = 0\end{aligned}$$

This results in a system of $d+1$ linear equations with $d+1$ unknowns that can be routinely solved (e.g. by using Gaussian elimination).

While this formulation is useful, it does not allow us to obtain a closed-form solution for $\mathbf{w}$ or discuss the existence or multiplicity of solutions. To address the first point we will exercise some matrix calculus, while the remaining points will be discussed later. We will first write the sum of square errors using the matrix notation as

$$\begin{aligned}\text{Err}(\mathbf{w}) &= (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y}) \\ &= \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2,\end{aligned}$$

where $\|\mathbf{v}\|_2 = \sqrt{\mathbf{v}^\top \mathbf{v}} = \sqrt{v_1^2 + v_2^2 + \dots v_n^2}$ is the length of vector $\mathbf{v}$; it is also called the L_2 norm. We can now formalize the *ordinary least-squares (OLS) linear regression problem* as

$$\mathbf{w}_{\text{ML}} = \arg\min_{\mathbf{w}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 .$$

We proceed by finding $\nabla \text{Err}(\mathbf{w})$ and $H_{\text{Err}(\mathbf{w})}$. The gradient function $\nabla \text{Err}(\mathbf{w})$ is a derivative of a scalar with respect to a vector. However, the intermediate steps of calculating the gradient require derivatives of vectors with respect to vectors (some of the rules of such derivatives are shown in Table B.1). Application of the rules from Table B.1 results in

$$\nabla \text{Err}(\mathbf{w}) = 2\mathbf{X}^\top \mathbf{X}\mathbf{w} - 2\mathbf{X}^\top \mathbf{y}$$

and, therefore, from $\nabla \text{Err}(\mathbf{w}) = \mathbf{0}$ we find that

$$\mathbf{w}_{\text{ML}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}. \tag{4.1}$$

The next step is to find the second derivative in order to ensure that we have not found a maximum (or saddle point). This results in

$$H_{\text{Err}(\mathbf{w})} = 2\mathbf{X}^\top \mathbf{X},$$

which is a positive semi-definite matrix (why? Consider that for any vector $\mathbf{x} \neq \mathbf{0}$, $\mathbf{x}^\top \mathbf{A}^\top \mathbf{A}\mathbf{x} = (\mathbf{A}\mathbf{x})^\top \mathbf{A}\mathbf{x} = \|\mathbf{A}\mathbf{x}\|_2^2 \geq 0$, with equality only if the columns of $\mathbf{A}$ are linearly dependent). Thus, we indeed have found a minimum. This is the global minimum because positive semi-definite Hessian implies convexity of $\text{Err}(\mathbf{w})$. Furthermore, if the columns of $\mathbf{x}$ are linearly independent, the Hessian is positive definite, which implies that the global minimum is unique. We can now express the predicted target values as

$$\begin{aligned} \hat{\mathbf{y}} &= \mathbf{X}\mathbf{w}_{\text{ML}} \\ &= \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}. \end{aligned}$$

The matrix $\mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top$ is called the *projection matrix*; see Section C.1 to understand how it projects $\mathbf{y}$ to the column space of $\mathbf{X}$.

Example 12: Consider again data set $\mathcal{D} = \{(1, 1.2), (2, 2.3), (3, 2.3), (4, 3.3)\}$ from Figure 4.1. We want to find the optimal coefficients of the least-squares fit for $f(x) = w_0 + w_1 x$ and then calculate the sum of squared errors on $\mathcal{D}$ after the fit.

The OLS fitting can now be performed using

$$\mathbf{x} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix}, \quad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 1.2 \\ 2.3 \\ 2.3 \\ 3.3 \end{bmatrix},$$

where a column of ones was added to $\mathbf{x}$ to allow for a non-zero intercept ($y = w_0$ when $x = 0$). Substituting $\mathbf{x}$ and $\mathbf{y}$ into Eq. (4.1) results in $\mathbf{w} = (0.7, 0.63)$ and the sum of square errors is $E(\mathbf{w}) = 0.223$. □

As seen in the example above, it is a standard practice to add a column of ones to the data matrix $\mathbf{x}$ in order to ensure that the fitted line, or generally a hyperplane, does not have

to pass through the origin of the coordinate system. This effect, however, can be achieved in other ways. Consider the first component of the gradient vector

$$\frac{\partial \text{Err}}{\partial w_0} = 2 \sum_{i=1}^{n} \left(\sum_{j=0}^{d} w_j x_{ij} - y_i \right) x_{i0} = 0$$

from which we obtain that

$$\sum_{i=1}^{n} w_0 = \sum_{i=1}^{n} y_i - \sum_{j=1}^{d} w_j \sum_{i=1}^{n} x_{ij}.$$

When all features (columns of $\mathbf{x}$) are normalized to have zero mean, i.e. when $\sum_{i=1}^{n} x_{ij} = 0$ for any column j, it follows that

$$w_0 = \frac{1}{n} \sum_{i=1}^{n} y_i.$$

We see now that if the target variable is normalized to the zero mean as well, it follows that $w_0 = 0$ and that the column of ones is not needed.

4.2.1 Weighted error function

In some applications it is useful to consider minimizing the weighted error function

$$\text{Err}(\mathbf{w}) = \sum_{i=1}^{n} c_i \left(\sum_{j=0}^{d} w_j x_{ij} - y_i \right)^2,$$

where $c_i > 0$ is a cost for data point i. Expressing this in a matrix form, the goal is to minimize $(\mathbf{X}\mathbf{w} - \mathbf{y})^\top \mathbf{C} (\mathbf{X}\mathbf{w} - \mathbf{y})$, where $\mathbf{C} = \text{diag}(c_1, c_2, \ldots, c_n)$. Using a similar approach as above, it can be shown that the weighted least-squares solution $\mathbf{w}_\text{C}$ can be expressed as

$$\mathbf{w}_\text{C} = \left(\mathbf{X}^\top \mathbf{C} \mathbf{X} \right)^{-1} \mathbf{X}^\top \mathbf{C} \mathbf{y}.$$

In addition, it can be derived that

$$\mathbf{w}_\text{C} = \mathbf{w}_\text{ML} + \left(\mathbf{X}^\top \mathbf{C} \mathbf{X} \right)^{-1} \mathbf{X}^\top (\mathbf{I} - \mathbf{C}) (\mathbf{X}\mathbf{w}_\text{ML} - \mathbf{y}),$$

where $\mathbf{w}_\text{ML}$ is provided by Eq. (4.1). We can see that the solutions are identical when $\mathbf{C} = \mathbf{I}$, but also when $\mathbf{X}\mathbf{w}_\text{ML} = \mathbf{y}$.

4.2.2 Predicting multiple outputs simultaneously

The extension to multiple outputs is straightforward, where now the target is an m-dimensional vector, $\mathbf{y} \in \mathbb{R}^m$, rather than a scalar, giving target matrix $\mathbf{Y} \in \mathbb{R}^{n \times m}$. Correspondingly, the weights $\mathbf{W} \in \mathbb{R}^{d \times m}$ to give $\mathbf{x}\mathbf{W} \in \mathbb{R}^m$, with error

$$\begin{aligned} E(\mathbf{W}) &= \|\mathbf{X}\mathbf{W} - \mathbf{Y}\|_F^2 = \sum_{i=1}^{n} \|\mathbf{X}_{i,:}\mathbf{W} - \mathbf{Y}_{i,:}\|_2^2 && \triangleright \text{ Frobenius norm} \\ &= \text{trace}\left((\mathbf{X}\mathbf{W} - \mathbf{Y})^\top (\mathbf{X}\mathbf{W} - \mathbf{Y}) \right) \end{aligned}$$

and solution

$$\mathbf{W}_{\text{ML}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Y}.$$

Exercise: Derive this solution, by taking partial derivatives or, preferably, by using gradient rules for matrix variables. A good resource for matrix gradients is the matrix cookbook.

4.2.3 Expectation and variance for the solution vector

Under the data generating model presented above, we shall now treat the solution vector (estimator) $\mathbf{w}_{\text{ML}}$ as a random variable and investigate its statistical properties. For each of the data points, we have $Y_i = \sum_{j=0}^{d} \omega_j X_{ij} + \varepsilon_i$, and use $\boldsymbol{\varepsilon} = (\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n)$ to denote a vector of i.i.d. random variables each drawn according to $\mathcal{N}(0, \sigma^2)$. Let us now look at the expected value (with respect to training data set D) for the weight vector $\mathbf{w}_{\text{ML}}$:

$$\begin{aligned}
\mathbb{E}[\mathbf{w}_{\text{ML}}(\mathcal{D})] &= \mathbb{E}\left[\left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \left(\mathbf{X}\boldsymbol{\omega} + \boldsymbol{\varepsilon}\right)\right] \\
&= \boldsymbol{\omega},
\end{aligned}$$

since $\mathbb{E}[\boldsymbol{\varepsilon}] = \mathbf{0}$. An estimator whose expected value is the true value of the parameter is called an *unbiased estimator*. The covariance matrix for the optimal set of parameters can be expressed as

$$\begin{aligned}
\text{Cov}[\mathbf{w}_{\text{ML}}(\mathcal{D})] &= \mathbb{E}\left[\left(\mathbf{w}_{\text{ML}}(\mathcal{D}) - \boldsymbol{\omega}\right)\left(\mathbf{w}_{\text{ML}}(\mathcal{D}) - \boldsymbol{\omega}\right)^\top\right] \\
&= \mathbb{E}\left[\mathbf{w}_{\text{ML}}(\mathcal{D})\mathbf{w}_{\text{ML}}(\mathcal{D})^\top\right] - \boldsymbol{\omega}\boldsymbol{\omega}^\top
\end{aligned}$$

Taking $\mathbf{X}^\dagger = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top$, we have

$$\begin{aligned}
\text{Cov}[\mathbf{w}_{\text{ML}}(\mathcal{D})] &= \mathbb{E}\left[\left(\boldsymbol{\omega} + \mathbf{X}^\dagger\boldsymbol{\varepsilon}\right)\left(\boldsymbol{\omega} + \mathbf{X}^\dagger\boldsymbol{\varepsilon}\right)^\top\right] - \boldsymbol{\omega}\boldsymbol{\omega}^\top \\
&= \boldsymbol{\omega}\boldsymbol{\omega}^\top + \mathbb{E}\left[\mathbf{X}^\dagger\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^\top\mathbf{X}^{\dagger\top}\right] - \boldsymbol{\omega}\boldsymbol{\omega}^\top
\end{aligned}$$

because $\mathbb{E}\left[\boldsymbol{\varepsilon}\right] = \mathbf{0}$, making $\mathbb{E}\left[\mathbf{X}^\dagger\boldsymbol{\varepsilon}\boldsymbol{\omega}^\top\right] = \mathbb{E}\left[\mathbf{X}^\dagger\right]\mathbb{E}\left[\boldsymbol{\varepsilon}\right]\boldsymbol{\omega}^\top = 0$. Now because the noise terms are independent of the inputs, i.e., $\mathbb{E}\left[\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^\top|\mathbf{X}\right] = \mathbb{E}\left[\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^\top\right] = \sigma^2\mathbf{I}$, we can use the law of total probability (also called the tower rule), to get

$$\begin{aligned}
\mathbb{E}\left[\mathbf{X}^\dagger\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^\top\mathbf{X}^{\dagger\top}\right] &= \mathbb{E}\left[\mathbb{E}\left[\mathbf{X}^\dagger\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^\top\mathbf{X}^{\dagger\top}|\mathbf{X}\right]\right] \\
&= \mathbb{E}\left[\mathbf{X}^\dagger\mathbb{E}\left[\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^\top|\mathbf{X}\right]\mathbf{X}^{\dagger\top}\right] \\
&= \sigma^2\mathbb{E}\left[\mathbf{X}^\dagger\mathbf{X}^{\dagger\top}\right].
\end{aligned}$$

Thus, we have

$$\text{Cov}[\mathbf{w}_{\text{ML}}(\mathcal{D})] = \sigma^2\mathbb{E}\left[(\mathbf{X}^\top\mathbf{X})^{-1}\right]$$

where we exploited the facts that $\mathbb{E}\left[\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^\top\right] = \sigma^2\mathbf{I}$ and that an inverse of a symmetric matrix is also a symmetric matrix. It can be shown that estimator $\mathbf{w}_{\text{ML}}(\mathcal{D}) = \mathbf{X}^\dagger\mathbf{y}$ is the one with the smallest variance among all unbiased estimators (Gauss-Markov theorem). These results are important not only because the estimated coefficients are expected to match the true coefficients of the underlying linear relationship, but also because the matrix inversion in

the covariance matrix suggests stability problems in cases of singular and nearly singular matrices. Numerical stability and sensitivity to perturbations will be discussed later.

To gain further insight into the ordinary linear regression solution, see an algebraic perspective in the appendix C.1. It provides more insights into uniqueness of the solution, and the space of possible solutions, and connects the linear regression optimization to solving systems.

4.3 Linear regression for non-linear problems

At first, it might seem that the applicability of linear regression and classification to real-life problems is greatly limited. After all, it is not clear whether it is realistic (most of the time) to assume that the target variable is a linear combination of features. Fortunately, the applicability of linear regression is broader than originally thought. The main idea is to apply a non-linear transformation to the data matrix $\mathbf{X}$ prior to the fitting step, which then enables a non-linear fit. Obtaining such a useful feature representation is a central problem in machine learning; we will discuss this in detail in Chapter 7. Here, we will first examine a simpler expanded representation that enables non-linear learning: polynomial curve fitting.

4.3.1 Polynomial curve fitting

We start with one-dimensional data. In OLS regression, we would look for the fit in the following form

$$f(x) = w_0 + w_1 x,$$

where x is the data point and $\mathbf{w} = (w_0, w_1)$ is the weight vector. To achieve a polynomial fit of degree p, we will modify the previous expression into

$$f(x) = \sum_{j=0}^{p} w_j x^j,$$

where p is the degree of the polynomial. We will rewrite this expression using a set of basis functions as

$$\begin{aligned} f(x) &= \sum_{j=0}^{p} w_j \phi_j(x) \\ &= \mathbf{w}^\top \boldsymbol{\phi}, \end{aligned}$$

where $\phi_j(x) = x^j$ and $\boldsymbol{\phi} = (\phi_0(x), \phi_1(x), \ldots, \phi_p(x))$. Applying this transformation to every data point in $\mathbf{x}$ results in a new data matrix $\boldsymbol{\Phi}$, as shown in Figure 4.2.

Following the discussion from Section 4.2, the optimal set of weights is now calculated as

$$\mathbf{w}_{\mathrm{ML}} = \left(\boldsymbol{\Phi}^\top \boldsymbol{\Phi}\right)^{-1} \boldsymbol{\Phi}^\top \mathbf{y}.$$

Example 13: In Figure 4.1 we presented an example of a data set with four data points. What we did not mention was that, given a set $\{x_1, x_2, x_3, x_4\}$, the targets were generated

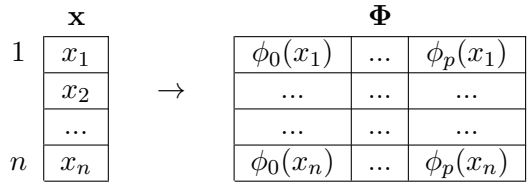


Figure 4.2: Transformation of an $n \times 1$ data matrix $\mathbf{x}$ into an $n \times (p+1)$ matrix $\mathbf{\Phi}$ using a set of basis functions ϕ_j, $j = 0, 1, \ldots, p$.

by using function $1 + \frac{x}{2}$ and then adding a measurement error $\mathbf{e} = (-0.3, 0.3, -0.2, 0.3)$. It turned out that the optimal coefficients $\mathbf{w}_{\text{ML}} = (0.7, 0.63)$ were close to the true coefficients $\boldsymbol{\omega} = (1, 0.5)$, even though the error terms were relatively significant. We will now attempt to estimate the coefficients of a polynomial fit with degrees $p = 2$ and $p = 3$. We will also calculate the sum of squared errors on $\mathcal{D}$ after the fit as well as on a large discrete set of values $x \in \{0, 0.1, 0.2, \ldots, 10\}$ where the target values will be generated using the true function $1 + \frac{x}{2}$.

Using a polynomial fit with degrees $p = 2$ and $p = 3$ results in $\mathbf{w}_2 = (0.575, 0.755, -0.025)$ and $\mathbf{w}_3 = (-3.1, 6.6, -2.65, 0.35)$, respectively. The sum of squared errors on $\mathcal{D}$ equals $E(\mathbf{w}_2) = 0.221$ and $E(\mathbf{w}_3) \approx 0$. Thus, the best fit is achieved with the cubic polynomial. However, the sum of squared errors on the outside data set reveal a poor generalization ability of the cubic model because we obtain $E(\mathbf{w}) = 26.9$, $E(\mathbf{w}_2) = 3.9$, and $E(\mathbf{w}_3) = 22018.5$. This effect is called *overfitting*. Broadly speaking, overfitting is indicated by a significant difference in fit between the data set on which the model was trained and the outside data set on which the model is expected to be applied (Figure 4.3). In this case, the overfitting occurred because the complexity of the model was increased considerably, whereas the size of the data set remained small.

One signature of overfitting is an increase in the magnitude of the coefficients. For example, while the absolute values of all coefficients in $\mathbf{w}$ and $\mathbf{w}_2$ were less than one, the values of the coefficients in $\mathbf{w}_3$ became significantly larger with alternating signs (suggesting overcompensation). We will discuss *regularization* in Section 4.4.2 as an approach to prevent this effect. □

Polynomial curve fitting is only one way of non-linear fitting because the choice of basis functions need not be limited to powers of x. Among others, non-linear basis functions that are commonly used are the sigmoid function

$$\phi_j(x) = \frac{1}{1 + e^{-\frac{x - \mu_j}{s_j}}}$$

or a Gaussian-style exponential function

$$\phi_j(x) = e^{-\frac{(x-\mu_j)^2}{2\sigma_j^2}},$$

where μ_j, s_j, and σ_j are constants to be determined. However, this approach works only for a one-dimensional input $\mathbf{x}$. For higher dimensions, this approach needs to be generalized using *radial basis functions*; see Section 7.1 for more details.

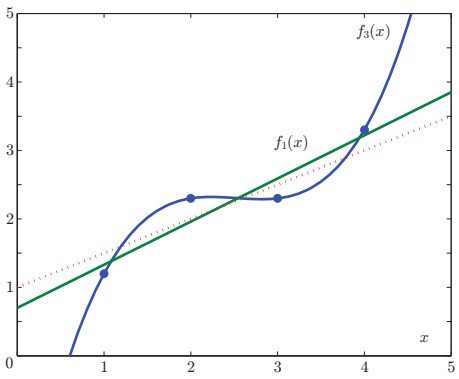


Figure 4.3: Example of a linear vs. polynomial fit on a data set shown in Figure 4.1. The linear fit, $f_1(x)$, is shown as a solid green line, whereas the cubic polynomial fit, $f_3(x)$, is shown as a solid blue line. The dotted red line indicates the target linear concept.

4.4 Practical considerations

In this section, we will discuss a few important considerations when implementing and using regression algorithms in practice.

4.4.1 Stability and sensitivity of the solutions

In practice, data sets include large numbers of features, which are sometimes identical, similar, or nearly linearly dependent. This causes $\mathbf{X}^\top\mathbf{X}$ to no longer be invertible and produces solutions that are sensitive to perturbations in $\mathbf{y}$ and $\mathbf{X}$. To see why, we will look at the *singular value decomposition* of $\mathbf{X}$. As with the previous linear algebra constructs, it allows us to easily examine properties of $\mathbf{X}$.

The singular value decomposition of $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$ for orthonormal matrices[1] $\mathbf{U} \in \mathbb{R}^{n\times n}, \mathbf{V} \in \mathbb{R}^{d\times d}$ and non-negative diagonal matrix $\mathbf{\Sigma} \in \mathbb{R}^{n\times d}$. The diagonal entries in $\mathbf{\Sigma}$ are the singular values; the number of non-zero singular values constitutes the rank of $\mathbf{X}$. Any matrix $\mathbf{X} \in \mathbb{R}^{n\times d}$ can be decomposed into its singular value decomposition, because any linear transformation can be decomposed into a rotation (multiplication by $\mathbf{V}^\top$), followed by a scaling (multiplication by $\mathbf{\Sigma}$), followed again by a rotation (multiplication by $\mathbf{U}$).

Now we can discuss the pseudo-inverse of $\mathbf{X}$ in terms of the singular value decomposition.

$$\mathbf{X}^\top\mathbf{X} = \mathbf{V}\mathbf{\Sigma}\mathbf{U}^\top\mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top = \mathbf{V}\mathbf{\Sigma}_d^2\mathbf{V}^\top \qquad \triangleright\, \mathbf{\Sigma}_d = \mathbf{\Sigma}(1:d, 1:d)$$

because $\mathbf{U}$ is orthonormal. The inverse of $\mathbf{X}^\top\mathbf{X}$ exists if $\mathbf{X}$ is full rank, i.e., $\mathbf{\Sigma}_d$ has no zeros on the diagonal, because $(\mathbf{X}^\top\mathbf{X})^{-1} = \mathbf{V}\mathbf{\Sigma}_d^{-2}\mathbf{V}^\top$. In the general case, however, the pseudo-inverse is still defined as the inverse of the non-zero singular values, $\mathbf{\Sigma}^\dagger$. This means that, even for $\mathbf{X}$ that is not full rank, we obtain the solution

$$\mathbf{w} = \mathbf{X}^\dagger\mathbf{y} = \mathbf{V}\mathbf{\Sigma}^\dagger\mathbf{U}^\top\mathbf{y} = \sum_{i=1}^{\text{rank of } \mathbf{X}} \frac{\mathbf{v}_i\mathbf{u}_i^\top}{\sigma_i}\mathbf{y}. \tag{4.2}$$

[1] An orthonormal matrix $\mathbf{U}$ is square matrix that satisfies $\mathbf{U}^\top\mathbf{U} = \mathbf{I}$ and $\mathbf{U}\mathbf{U}^\top = \mathbf{I}$

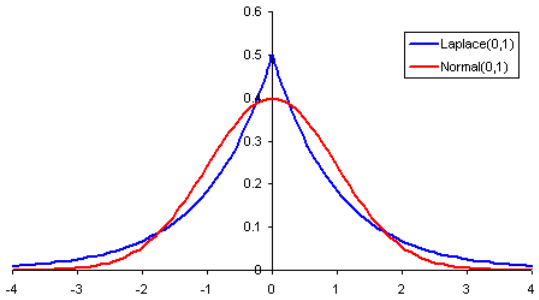


Figure 4.4: A comparison between Gaussian and Laplace priors. Both prefers values to be near zero, but the Laplace prior more strongly prefers the values to equal zero.

Notice that for full-rank $\mathbf{X}$,

$$(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top = \mathbf{V}\boldsymbol{\Sigma}_d^{-2}\mathbf{V}^\top\mathbf{V}\boldsymbol{\Sigma}\mathbf{U}^\top = \mathbf{V}\boldsymbol{\Sigma}_d^{-2}\boldsymbol{\Sigma}\mathbf{U}^\top = \mathbf{V}\boldsymbol{\Sigma}_d^{-1}\mathbf{U}^\top$$

which matches the definition of the pseudo-inverse using the singular value decomposition for non-full rank matrices.

The solution in Equation (4.2) makes it clear why the solution can be sensitive to perturbations. For small singular values, due to being nearly linearly dependent, σ_i^{-1} is large and amplifies any changes in $\mathbf{y}$. Moreover, for different samples in $\mathbf{X}$, and for different numbers of samples, we will see different small singular values, which will again strongly affect the solution.

A common strategy to deal with this instability is to drop or truncate small singular values. This is a form of regularization, which we discuss next.

4.4.2 Regularization

So far, we have discussed linear regression in terms of maximum likelihood. But, as before, we can also propose a MAP objective. Instead of specifying no prior over $\mathbf{w}$, we can select a prior to help *regularize* overfitting to the observed data. We will discuss two common priors (regularizers): the Gaussian prior (ℓ_2 norm) and the Laplace prior (ℓ_1 norm), shown in Figure 4.4.

Taking the log of the zero-mean Gaussian prior, $\mathcal{N}(\mathbf{0}, \lambda^{-1}\mathbf{I})$, we get

$$-\ln p(\mathbf{w}) = \ln(2\pi|\lambda^{-1}\mathbf{I}|) + \frac{\mathbf{w}^\top\mathbf{w}}{2\lambda^{-1}} = \ln(2\pi) - d\ln(\lambda) + \frac{\lambda}{2}\mathbf{w}^\top\mathbf{w}.$$

because $|\lambda^{-1}\mathbf{I}| = \lambda^{-d}$, where $|\mathbf{A}|$ is the determinant of the matrix $\mathbf{A}$. As before, we can drop the first constant which does not affect the selection of $\mathbf{w}$, and now combine the negative log-likelihood and the negative log prior to get the following ridge regression problem:

$$\mathrm{Err}(\mathbf{w}) = (\mathbf{X}\mathbf{w} - \mathbf{y})^\top(\mathbf{X}\mathbf{w} - \mathbf{y}) + \lambda\mathbf{w}^\top\mathbf{w} \qquad \triangleright\ \|\mathbf{w}\|_2^2 = \mathbf{w}^\top\mathbf{w}$$

where λ is a user-selected parameter that is called the *regularization parameter*. The idea is to penalize weight coefficients that are too large; the larger the λ, the more large weights are penalized. If we solve this equation in a similar manner as before, we obtain

$$\mathbf{w}_{\mathrm{MAP}} = (\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{y}.$$

This has the nice effect of shifting the squared singular values in Σ_d^2 by λ, removing stability issues with dividing by small singular values, as long as λ is itself large enough.

Similarly, if we choose a Laplace distribution, we get an ℓ_1 penalized loss

$$\text{Err}(\mathbf{w}) = (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y}) + \lambda \|\mathbf{w}\|_1$$

which is often called the Lasso. As with the ℓ_2 regularizer for ridge regression, this regularizer penalized large values in $\mathbf{w}$. However, it also produces more sparse solutions, where entries in $\mathbf{w}$ are zero. This has the effect of feature selection, because zeroing entries in $\mathbf{w}$ is equivalent to removing the corresponding feature.

Notice, however, that for the Lasso we no longer have a closed form solution. Instead, we will use gradient descent to compute a solution to $\mathbf{w}$. In Algorithm 1, we provide a gradient descent algorithm for the incremental update with the ℓ_1 regularizer. A reasonable approach would be to take the gradient of ℓ_1, and modify the gradient descent update with this additional component. The ℓ_1 regularizer, however, is non-differentiable at 0. Instead, we provide an algorithm that is more effective in practice. The idea is simple: use gradient descent for the smooth component of the optimization (the error term $\|\mathbf{X}\mathbf{w}-\mathbf{y}\|_2^2$), and then for values in $\mathbf{w}$ that are close to zero, set them to zero. This thresholding idea, though simple, is a theoretically sound approach for optimizing with the non-smooth ℓ_1. This thresholding operator is called the proximal operator, and can be seen as a projection operator. Each time $\mathbf{w}$ is updated with the gradient, it moves it away from a sparse solution; the proximal operator then projects $\mathbf{w}$ back onto the space of sparse solutions. The proximal operator for ℓ_1 is applied element-wise to $\mathbf{w}$, and so is defined on each $\mathbf{w}_i$ as, with stepsize η and regularization parameter λ,

$$\text{prox}_{\eta\lambda\ell_1}(\mathbf{w}_i) = \begin{cases} \mathbf{w}_i - \eta\lambda & \text{if } \mathbf{w}_i > \eta\lambda; \\ 0 & \text{if } |\mathbf{w}_i| \leq \eta\lambda; \\ \mathbf{w}_i + \eta\lambda & \text{if } \mathbf{w}_i < -\eta\lambda. \end{cases}$$

Algorithm 1: Batch gradient descent for ℓ_1 regularized linear regression $(\mathbf{X}, \mathbf{y}, \lambda)$

$\mathbf{w} \leftarrow \mathbf{0} \in \mathbb{R}^d$
err $\leftarrow \infty$
tolerance $\leftarrow 10e^{-4}$
$XX \leftarrow \frac{1}{n}\mathbf{X}^\top\mathbf{X}$
$Xy \leftarrow \frac{1}{n}\mathbf{X}^\top\mathbf{y}$
$\eta \leftarrow 1/(2\|XX\|_2)$
while $|\text{Err}(\mathbf{w}) - \text{err}| >$ tolerance **do**
    err $\leftarrow \text{Err}(\mathbf{w})$
    // The proximal operator projects back into the space of sparse solutions given by ℓ_1
    $\mathbf{w} \leftarrow \text{prox}_{\eta\lambda\ell_1}(\mathbf{w} - \eta XX\mathbf{w} + \eta Xy)$
return $\mathbf{w}$

4.4.3 Handling big data sets

One common approach to handling big datasets is to use *stochastic approximation*, where samples are processed incrementally. To see how this would be done, let us revisit the

gradient of the error function, $\nabla \text{Err}(\mathbf{w})$. We obtained a closed form solution for $\nabla \text{Err}(\mathbf{w}) = \mathbf{0}$; however, for many other error functions, solving for $\nabla \text{Err}(\mathbf{w}) = \mathbf{0}$ in a closed form way is not possible. Instead, we start at some initial $\mathbf{w}_0$ (typically random), and then step in the direction of the negative of the gradient until we reach a local minimum. This approach is called *gradient descent* and is summarized in Algorithm 2. Notice that here the gradient is normalized by the number of samples n, as $\mathbf{X}^\top(\mathbf{X}\mathbf{w} - \mathbf{y})$ grows with the number of samples and makes it more difficult to select the stepsize.

Algorithm 2: Batch Gradient Descent$(\text{Err}, \mathbf{X}, \mathbf{y})$

// A non-optimized, basic implementation of batch gradient descent
$\mathbf{w} \leftarrow$ random vector in $\mathbb{R}^d$
$\text{err} \leftarrow \infty$
$\text{tolerance} \leftarrow 10e^{-4}$
while $|\text{Err}(\mathbf{w}) - \text{err}| > \text{tolerance}$ **do**
  $\text{err} \leftarrow \text{Err}(\mathbf{w})$
  $\mathbf{g} \leftarrow \nabla \text{Err}(\mathbf{w})$ ▷ for linear regression, $\nabla \text{Err}(\mathbf{w}) = \frac{1}{n}\mathbf{X}^\top(\mathbf{X}\mathbf{w} - \mathbf{y})$
  // The step-size η could be chosen by line-search
  $\eta \leftarrow \text{line search}(\mathbf{w}, \mathbf{g}, \text{Err})$
  $\mathbf{w} \leftarrow \mathbf{w} - \eta\mathbf{g}$
return $\mathbf{w}$

For a large number of samples n, however, computing the gradient across all samples can be expensive or infeasible. An alternative is to approximate the gradient less accurately with fewer samples. In stochastic approximation, we typically approximate the gradient with one sample[2], as in Algorithm 3. Though this approach may appear to be too much of an approximation, there is a long theoretical and empirical history indicating its effectiveness (see for example [5, 4]). With ever increasing data-set size for many scenarios, the generality of stochastic approximation makes it arguably the modern approach to dealing with big data. For specialized scenarios, there are of course other approaches. For one example, see [13].

Algorithm 3: Stochastic Gradient Descent$(\text{Err}, \mathbf{X}, \mathbf{y})$

$\mathbf{w} \leftarrow$ random vector in $\mathbb{R}^d$
for $i = 1, \ldots$ number of epochs **do**
  Shuffle data points from $1, \ldots, n$
  for $t = 1, \ldots, n$ **do**
    $\mathbf{g}_t \leftarrow \nabla \text{Err}(\mathbf{w})$ ▷ for linear regression, $\nabla \text{Err}_t(\mathbf{w}) = (\mathbf{x}_t^\top \mathbf{w} - y_t)\mathbf{x}_t$
    // For convergence, we need step-size η_t to decrease with time
    // For example, a common choice is $\eta_t = \eta_0 t^{-1}$ or
    // $\eta_t = \eta_0 t^{-1/2}$ for some initial η_0, such as $\eta_0 = 1.0$.
    // In practice, it is common to pick a fixed, small stepsize.
    $\mathbf{w} \leftarrow \mathbf{w} - \eta_t \mathbf{g}_t$
return $\mathbf{w}$

[2]Mini-batches are a way to obtain a better approximation but remain efficient.

Chapter 5

Generalized Linear Models

In previous sections, we saw that the statistical framework provided valuable insights into linear regression, especially with respect to explicitly stating most of the assumptions in the system (we will see the full picture only when Bayesian formulation is used). These assumptions were necessary to rigorously estimate parameters of the model, which could then be subsequently used for prediction on previously unseen data points.

In this section, we introduce generalized linear models (GLMs) which extend ordinary least-squares regression beyond Gaussian probability distributions and linear dependencies between the features and the target. This generalization will also introduce you to a broader range of loss functions, called Bregman divergences.

We shall first revisit the main points of the ordinary least-squares regression. There, we assumed that a set of i.i.d. data points with their targets $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ were drawn according to some distribution $p(\mathbf{x}, y)$. We also assumed that an underlying relationship between the features and the target was linear, i.e.

$$Y = \sum_{j=0}^{d} \omega_j X_j + \varepsilon,$$

where $\boldsymbol{\omega}$ was a set of unknown weights and ε was a zero-mean normally distributed random variable with variance σ^2. In order to simplify generalization, we will slightly reformulate this model. In particular, it will be useful to separate the underlying linear relationship between the features and the target from the fact that Y was normally distributed. That is, we will write that

1. $E[y|\mathbf{x}] = \boldsymbol{\omega}^\top \mathbf{x}$
2. $p(y|\mathbf{x}) = \mathcal{N}(\mu, \sigma^2)$

with $\mu = \boldsymbol{\omega}^\top \mathbf{x}$ connecting the two expressions. This way of formulating linear regression will allow us (i) to generalize the framework to non-linear relationships between the features and the target as well as (ii) to use the error distributions other than Gaussian.

5.1 Loglinear link and Poisson distribution

Let us start with an example. Assume that data points correspond to cities in the world (described by some numerical features) and that the target variable is the number of sunny days observed in a particular year. To establish the GLM model, we will assume (1) a loglinear link between the expectation of the target and linear combination of features, and (2) the Poisson distribution for the target variable. We summarize these assumptions as follows

1. $\log(E[y|\mathbf{x}]) = \boldsymbol{\omega}^\top \mathbf{x}$
2. $p(y|\mathbf{x}) = \text{Poisson}(\lambda)$

where $\lambda > 0$ is the parameter (mean and variance) of the Poisson distribution. Exploiting the fact that $E[y|\mathbf{x}] = \lambda$, we connect the two formulas using $\lambda = e^{\boldsymbol{\omega}^\top \mathbf{x}}$. In fact, because $\lambda \in \mathbb{R}^+$ and $\boldsymbol{\omega}^\top \mathbf{x} \in \mathbb{R}$, it is not appropriate to use a linear link between $E[y|\mathbf{x}]$ and $\boldsymbol{\omega}^\top \mathbf{x}$ (i.e. $E[y|\mathbf{x}] = \boldsymbol{\omega}^\top \mathbf{x}$). The link function adjusts the range of the linear combination of features (so-called systematic component) to the domain of the parameters (here, mean) of the probability distribution.

We provide a compact summary of the above assumptions via a probability distribution for the target; i.e. $p(y|\mathbf{x}) = \text{Poisson}(e^{\boldsymbol{\omega}^\top \mathbf{x}})$. We express this as

$$p(y|\mathbf{x}) = \frac{e^{\boldsymbol{\omega}^\top \mathbf{x} y} \cdot e^{-e^{\boldsymbol{\omega}^\top \mathbf{x}}}}{y!}$$

for any $y \in \mathbb{N}$. We will now use the maximum likelihood estimation to find the parameters of the regression model. As in previous sections, the likelihood function has the form of the probability distribution, where the data set is observed and the parameters are unknown. Hence, the log-likelihood function has the form

$$ll(\mathbf{w}) = \sum_{i=1}^{n} \mathbf{w}^\top \mathbf{x}_i y_i - \sum_{i=1}^{n} e^{\mathbf{w}^\top \mathbf{x}_i} - \sum_{i=1}^{n} y_i!$$

It is easy to show that $\nabla ll(\mathbf{w}) = \mathbf{0}$ does not have a closed-form solution. Therefore, we will use the Newton-Raphson method in which we must first analytically find the gradient vector $\nabla ll(\mathbf{w})$ and the Hessian matrix $H_{ll(\mathbf{w})}$. We start by deriving the j-th element of the gradient

$$\begin{aligned}
\frac{\partial ll(\mathbf{w})}{\partial w_j} &= \sum_{i=1}^{n} x_{ij} y_i - \sum_{i=1}^{n} e^{\mathbf{w}^\top \mathbf{x}_i} x_{ij} \\
&= \sum_{i=1}^{n} x_{ij} \cdot \left(y_i - e^{\mathbf{w}^\top \mathbf{x}_i} \right) \\
&= \mathbf{f}_j^\top \cdot (\mathbf{y} - \mathbf{c}),
\end{aligned}$$

where $\mathbf{f}_j^\top$ is the j-th column of $\mathbf{x}$ and $\mathbf{c}$ is a vector with elements $c_i = e^{\mathbf{w}^\top \mathbf{x}_i}$. The gradient of the likelihood function can now be expressed as

$$\nabla ll(\mathbf{w}) = \mathbf{X}^\top \cdot (\mathbf{y} - \mathbf{c}). \tag{5.1}$$

Note that $\mathbf{c}$ stores a set of predictions for each of the data points, and thus, $\mathbf{y} - \mathbf{c}$ is an error vector. The second partial derivative of the likelihood function can be derived as

$$\begin{aligned}
\frac{\partial^2 ll(\mathbf{w})}{\partial w_j \partial w_d} &= -\sum_{i=1}^{n} x_{ij} \cdot e^{\mathbf{w}^\top \mathbf{x}_i} \cdot x_{ik} \\
&= -\mathbf{f}_j^\top \cdot \mathbf{C} \cdot \mathbf{f}_d,
\end{aligned}$$

where $\mathbf{C}$ is an n-by-n diagonal matrix with $c_{ii} = e^{\mathbf{w}^\top \mathbf{x}_i}$. The Hessian matrix can now be calculated as

$$H_{ll(\mathbf{w})} = -\mathbf{X}^\top \cdot \mathbf{C} \cdot \mathbf{X}. \tag{5.2}$$

which is a negative semi-definite matrix. Substituting Eq. (5.1) and Eq. (5.2) into the Newton-Raphson formula results in the following weight update rule

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} + \left(\mathbf{X}^\top \cdot \mathbf{C}^{(t)} \cdot \mathbf{X}\right)^{-1} \cdot \mathbf{X}^\top \cdot \left(\mathbf{y} - \mathbf{c}^{(t)}\right),$$

where $\mathbf{c}^{(t)}$ and $\mathbf{C}^{(t)}$ are calculated using the weight vector $\mathbf{w}^{(t)}$. The initial set of weights $\mathbf{w}^{(0)}$ can be set randomly.

5.2 Exponential family of distributions

In the previous section, we used a specific example to illustrate how to generalize beyond Gaussian distributions. The approach more generally extends to any exponential family distribution. For simplicity, here we focus on the natural exponential family, which is sufficient for most generalized linear models. The natural exponential family is a class of probability distributions with the following form

$$p(x|\theta) = \exp\left(\theta x - a(\theta) + b(x)\right)$$

where $\theta \in \mathbb{R}$ is the parameter to the distribution, $a : \mathbb{R} \to \mathbb{R}$ is a log-normalizer function and $b : \mathbb{R} \to \mathbb{R}$ is a function of only x that will typically be ignored in our optimization because it is not a function of θ. Many of the often encountered (families of) distributions are members of the exponential family; e.g. exponential, Gaussian, Gamma, Poisson, or the binomial distributions. Therefore, it is useful to generically study the exponential family to better understand commonalities and differences between individual member functions.

Example 14: The Poisson distribution can be expressed as

$$p(x|\lambda) = \exp\left(x \log \lambda - \lambda - \log x!\right),$$

where $\lambda \in \mathbb{R}^+$ and $\mathcal{X} = \mathbb{N}_0$. Thus, $\theta = \log \lambda$, $a(\theta) = e^\theta$, and $b(x) = -\log x!$. □

Now let us get some further insight into the properties of the exponential family parameters and why this class is convenient for estimation. The function $a(\theta)$ is typically called the log-partitioning function or simply a log-normalizer. It is called this because

$$a(\theta) = \log \int_{\mathcal{X}} \exp\left(\theta x + b(x)\right) dx$$

and so plays the role of ensuring that we have a valid density: $\int_{\mathcal{X}} p(x)dx = 1$. Importantly, for many common GLMs, the derivative of a corresponds to the inverse of the link function. For example, for Poisson regression, the link function $g(\theta) = \log(\theta)$, and the derivative of a is e^θ, which is the inverse of g. Therefore, as we discuss below in Section 5.5, the log-normalizer for an exponential family informs what link g should be used (or correspondingly the transfer $f = g^{-1}$).

The properties of this log-normalizer are also key for estimation of generalized linear models. It can be derived that

$$\begin{aligned}\frac{\partial a(\theta)}{\partial \theta} &= \mathbb{E}[X] \\ \frac{\partial^2 a(\theta)}{\partial \theta^2} &= \mathrm{V}[X]\end{aligned}$$

These properties are useful for estimating parameters of the distribution. For example, let us consider a data set of observations $\mathcal{D} = \{x_i\}_{i=1}^n$ and look at the log-likelihood function

$$\begin{aligned}ll(\theta) &= \log \prod_{i=1}^n e^{\theta x_i - a(\theta) + b(x_i)} \\ &= \sum_{i=1}^n \theta x_i - n a(\theta) + \sum_{i=1}^n b(x_i).\end{aligned}$$

Maximizing the likelihood involves calculating the gradient function

$$\nabla ll(\theta) = \sum_{i=1}^n x_i - n \nabla a(\theta).$$

Setting the gradient to zero results in

$$\nabla a(\theta) = \frac{1}{n} \sum_{i=1}^n x_i$$

By combining the previous expressions we see that the likelihood is maximized when the gradient function of the log-normalizer equals the sample mean of x. This result is important because it provides a general expression for estimating the parameters of all distributions in the exponential family.

5.3 Formalizing generalized linear models

We shall now formalize the generalized linear models. The two key components of GLMs can be expressed as

1. $g(E[y|\mathbf{x}]) = \boldsymbol{\omega}^\top \mathbf{x}$ or $E[y|\mathbf{x}] = f(\boldsymbol{\omega}^\top \mathbf{x})$ where $g = f^{-1}$
2. $p(y|\mathbf{x}) \in$ Exponential Family

Here, $g(\cdot)$ is called the link function between the linear combination of the features and parameters of the distribution. On the one hand, the link function adjusts the range of $\boldsymbol{\omega}^\top \mathbf{x}$ to the domain of Y (because of this relationship, link functions are usually not selected independently of the distribution for Y). On the other hand, it also provides a mechanism for a non-linear relationship between the features and the target. While the nature of this non-linear relationship is limited (the features enter the system via a linear combination with the parameters) there is still an important flexibility they provide for modeling. Similarly, the generalization to the exponential family from the Gaussian distribution used in ordinary

least-squares regression, allows us to model a much wider range of target functions. The choice of the link function and the probability distribution is data dependent.

Generally, there is no guarantee of a closed-form solution for $\mathbf{w}$. Therefore, GLM formulations usually use iterative techniques derived from the Taylor approximation of the log-likelihood. Hence, a single mechanism can be used for a wide range of link functions and probability distributions. Let us write the log-likelihood

$$\begin{aligned} ll(\mathbf{w}) &= \log \prod_{i=1}^{n} e^{\theta y_i - a(\theta) + b(y_i)} \\ &= \sum_i \theta y_i - n a(\theta) + \sum_i b(y_i) \\ &= \sum_i ll_i(\mathbf{w}) \end{aligned}$$

and also find the elements of its gradient

$$\frac{\partial ll_i(\mathbf{w})}{\partial w_j} = \frac{\partial \theta}{\partial w_j} y_i - \frac{\partial a(\theta)}{\partial w_j}$$

which can be used to easily calculate the update rules of the optimization. Interestingly, the standard versions of the GLM from the literature do not use the full version of the Newton-Raphson algorithm with the Hessian matrix. Instead, Gauss-Newton and other types of solutions are considered and are generally called iteratively reweighted least-squares (IRLS) algorithms in the statistical literature.

5.4 Logistic regression

One of the most popular uses of GLMs is a combination of a Bernoulli distribution with a logit link function, which is useful for classification. This framework is frequently encountered and is called logistic regression. We summarize the logistic regression model as follows

1. $\text{logit}(E[y|\mathbf{x}]) = \boldsymbol{\omega}^\top \mathbf{x}$
2. $p(y|\mathbf{x}) = \text{Bernoulli}(\alpha)$

where $\text{logit}(x) = \ln \frac{x}{1-x}$, $y \in \{0, 1\}$, and $\alpha \in (0, 1)$ is the parameter (mean) of the Bernoulli distribution. It follows that

$$E[y|\mathbf{x}] = \frac{1}{1 + e^{-\boldsymbol{\omega}^\top \mathbf{x}}} = \sigma(\boldsymbol{\omega}^\top \mathbf{x})$$

and

$$p(y|\mathbf{x}) = \left(\frac{1}{1 + e^{-\omega^\top \mathbf{x}}}\right)^y \left(1 - \frac{1}{1 + e^{-\omega^\top \mathbf{x}}}\right)^{1-y}$$

where $\sigma : \mathbb{R} \to [0, 1]$ is called the sigmoid function. Given a data set $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$, where $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \{0, 1\}$, the parameters of the model $\mathbf{w}$ can be found by maximizing the likelihood function.

5.5 [Advanced] Connection to Bregman divergences

We have discussed that the link g or transfer function f is chosen to reflect the range of the output variable y. However, the choice should have other properties as well. In particular, we would like to ensure that the g provides a smooth, convex negative log-likelihood, to simplify optimization. Usefully, the parameter a of the exponential family distribution provides us with just such a choice: $f = \nabla a$. This choice in fact provides a Bregman divergence that corresponds to the negative log-likelihood of a natural exponential family: $D_a(x||g(\theta)) = -\ln p(x|\theta)$. See [16, Section 2.2] for more details about this relationship. For $\theta = \mathbf{x}^\top \mathbf{w}$, the generic log-likelihood for the exponential family is

$$\begin{aligned}\frac{\partial ll_i(\mathbf{w})}{\partial w_j} &= \frac{\partial \theta}{\partial w_j} y_i - \frac{\partial a(\theta)}{\partial w_j} \\ &= (y_i - f(\theta)) x_j\end{aligned}$$

The same result about the mean minimizer being optimal has been shown for Bregman divergences [2]. For any Bregman divergence, $\text{argmin}_{\hat{x}} \sum_{i=1}^n D_a(x_i||\theta) = \frac{1}{n}\sum_{i=1}^n x_i$, i.e., the optimal solution is the sample mean. Therefore, when optimizing the log-likelihood for a natural exponential family, we obtain a corresponding Bregman divergence and the minimizer $g^{-1}(\boldsymbol{\theta})$ corresponds to the mean of the data.

It is important to note that the chosen link does not necessarily have to correspond to the derivative of a. Rather, this provides a mechanism for ensuring a nice loss function (since Bregman divergences have nice properties). However, this does not mean that any other link will necessarily result in an undesirable loss function.

Chapter 6

Linear Classifiers

Suppose we are interested in building a linear classifer $f : \mathbb{R}^d \to \{-1, +1\}$. Linear classifiers try to find the relationship between inputs and outputs by constructing a linear function (a point, a line, a plane or a hyperplane) that splits $\mathbb{R}^d$ into two half-spaces. The two half-spaces act as decision regions for the positive and negative examples, respectively. Given a data set $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ consisting of positive and negative examples, there are many ways in which linear classifiers can be constructed. For example, a training algorithm may explicitly work to position the decision surface in order to separate positive and negative examples according to some problem-relevant criteria; e.g. it may try to minimize the fraction of examples on the incorrect side of the decision surface. Alternatively, the goal of the training algorithm may be to directly estimate the posterior distribution $p(y|\mathbf{x})$, in which case the algorithm is more likely to rely on the formal parameter estimation principles; e.g. it may maximize the likelihood. An example of a classifier with a linear decision surface is shown in Figure 6.1.

To simplify the formalism in the following sections, we will add a component $x_0 = 1$ to each input $(x_1, \ldots, x_d)$. This extends the input space to $\mathcal{X} = \mathbb{R}^{d+1}$ but, fortunately, it also leads us to a simplified notation in which the decision boundary in $\mathbb{R}^d$ can be written as $\mathbf{w}^\top \mathbf{x} = 0$, where $\mathbf{w} = (w_0, w_1, \ldots, w_d)$ is a set of weights and $\mathbf{x} = (x_0 = 1, x_1, \ldots, x_d)$ is any element of the input space. Neverthless, we should remember that the actual inputs are d-dimensional.

Earlier in the introductory remarks, we presented a classifier as a function $f : \mathcal{X} \to \mathcal{Y}$ and have transformed the learning problem into approximating $p(y|\mathbf{x})$. In the case of

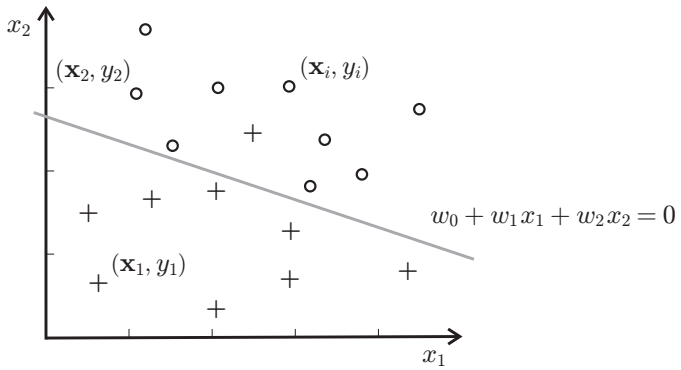


Figure 6.1: A data set in $\mathbb{R}^2$ consisting of nine positive and nine negative examples. The gray line represents a linear decision surface in $\mathbb{R}^2$. The decision surface does not perfectly separate positives from negatives.

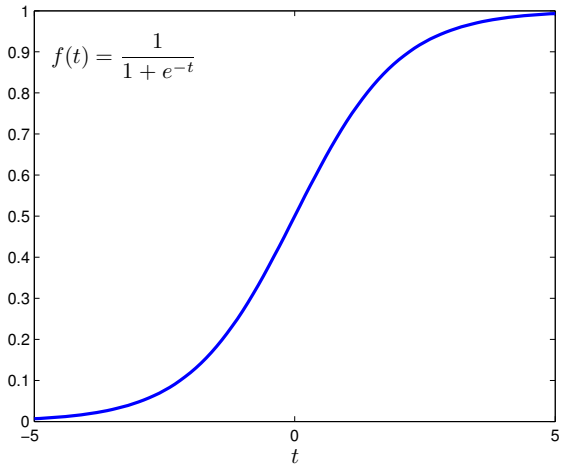


Figure 6.2: Sigmoid function in $[-5, 5]$ *interval.*

linear classifiers, our flexibility is restricted because our method must learn the posterior probabilities $p(y|\mathbf{x})$ and at the same time have a linear decision surface in $\mathbb{R}^d$. This, however, can be achieved if $p(y|\mathbf{x})$ is modeled as a monotonic function of $\mathbf{w}^\top\mathbf{x}$; e.g. $\tanh(\mathbf{w}^\top\mathbf{x})$ or $(1+e^{-\mathbf{w}^\top\mathbf{x}})^{-1}$. Of course, a model trained to learn posterior probabilities $p(y|\mathbf{x})$ can be seen as a function $g : \mathcal{X} \to [0, 1]$. Then, the conversion from g to f is a straightforward application of the maximum a posteriori principle: the predicted output is positive if $g(\mathbf{x}) \geq 0.5$ and negative if $g(\mathbf{x}) < 0.5$.

6.1 Logistic regression

Let us consider binary classification in $\mathbb{R}^d$, where $\mathcal{X} = \mathbb{R}^{d+1}$ and $\mathcal{Y} = \{0, 1\}$. The basic idea for many classification approaches is to hypothesize a closed-form representation for the posterior probability that the class label is positive and learn parameters $\mathbf{w}$ from data. In logistic regression, this relationship can be expressed as

$$P(Y = 1|\mathbf{x}, \mathbf{w}) = \frac{1}{1 + e^{-\mathbf{w}^\top\mathbf{x}}}, \tag{6.1}$$

which is a monotonic function of $\mathbf{w}^\top\mathbf{x}$. Function $\sigma(t) = \left(1 + e^{-t}\right)^{-1}$ is called the sigmoid function or the logistic function and is plotted in Figure 6.2.

6.1.1 Predicting class labels

For a previously unseen data point $\mathbf{x}$ and a set of coefficients $\mathbf{w}^*$ found from Eq. (6.4) or Eq. (6.11), we simply calculate the posterior probability as

$$P(Y = 1|\mathbf{x}, \mathbf{w}^*) = \frac{1}{1 + e^{-\mathbf{w}^{*T}\cdot\mathbf{x}}}.$$

If $P(Y = 1|\mathbf{x}, \mathbf{w}^*) \geq 0.5$ we conclude that data point $\mathbf{x}$ should be labeled as positive ($\hat{y} = 1$). Otherwise, if $P(Y = 1|\mathbf{x}, \mathbf{w}^*) < 0.5$, we label the data point as negative ($\hat{y} = 0$). Thus,

the predictor maps a $(d+1)$-dimensional vector $\mathbf{x} = (x_0 = 1, x_1, \ldots, x_d)$ into a zero or one. Note that $P(Y = 1|\mathbf{x}, \mathbf{w}^*) \geq 0.5$ only when $\mathbf{w}^\top \mathbf{x} \geq 0$. The expression $\mathbf{w}^\top \mathbf{x} = 0$ represents equation of a hyperplane that separates positive and negative examples. Thus, the logistic regression model is a linear classifier.

6.1.2 Maximum conditional likelihood estimation

To frame the learning problem as parameter estimation, we will assume that the data set $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ is an i.i.d. sample from a fixed but unknown probability distribution $p(\mathbf{x}, y)$. Even more specifically, we will assume that the data generating process randomly draws a data point $\mathbf{x}$, a realization of the random vector $(X_0 = 1, X_1, \ldots, X_d)$, according to $p(\mathbf{x})$ and then sets its class label Y according to the Bernoulli distribution

$$\begin{aligned} p(y|\mathbf{x}) &= \begin{cases} \left(\frac{1}{1+e^{-\boldsymbol{\omega}^\top \mathbf{x}}}\right)^y & \text{for } y = 1 \\ \left(1 - \frac{1}{1+e^{-\boldsymbol{\omega}^\top \mathbf{x}}}\right)^{1-y} & \text{for } y = 0 \end{cases} \\ &= \sigma(\mathbf{x}^\top \mathbf{w})^y (1 - \sigma(\mathbf{x}^\top \mathbf{w}))^{1-y} \end{aligned} \tag{6.2}$$

where $\boldsymbol{\omega} = (\omega_0, \omega_1, \ldots, \omega_d)$ is a set of unknown coefficients we want to recover (or learn) from the observed data $\mathcal{D}$. Based on the principles of parameter estimation, we can estimate $\boldsymbol{\omega}$ by maximizing the conditional likelihood of the observed class labels $\mathbf{y} = (y_1, y_2, \ldots, y_n)$ given the inputs $\mathbf{X} = (\mathbf{x}_1^\top, \mathbf{x}_2^\top, \ldots, \mathbf{x}_n^\top)$.

As with the previous maximum likelihood estimation, we shall first write the conditional likelihood function $p(\mathbf{y}|\mathbf{X}, \mathbf{w})$, or simply $l(\mathbf{w})$, as

$$l(\mathbf{w}) = \prod_{i=1}^n p(y_i|\mathbf{x}_i, \mathbf{w}). \tag{6.3}$$

This function can be thought of as the probability of observing a set of labels $\mathbf{y}$ given the set of data points $\mathbf{X}$ and the particular set of coefficients $\mathbf{w}$. The parameter vector that maximizes the likelihood is

$$\begin{aligned} \mathbf{w}_{\text{ML}} &= \arg\max_{\mathbf{w}} \{l(\mathbf{w})\} \\ &= \arg\max_{\mathbf{w}} \left\{ \prod_{i=1}^n p(y_i|\mathbf{x}_i, \mathbf{w}) \right\} \qquad (6.4) \\ &= \prod_{i=1}^n \left(\frac{1}{1+e^{-\mathbf{w}^\top \mathbf{x}_i}} \right)^{y_i} \cdot \left(1 - \frac{1}{1+e^{-\mathbf{w}^\top \mathbf{x}_i}} \right)^{1-y_i}. \qquad (6.5) \end{aligned}$$

As before, because log is a monotonic function, maximizing Eq. (6.5) is equivalent to maximizing the log-likelihood function $ll(\mathbf{w}) = \log(l(\mathbf{w}))$

$$ll(\mathbf{w}) = \sum_{i=1}^n \left(y_i \cdot \log\left(\frac{1}{1+e^{-\mathbf{w}^\top \mathbf{x}_i}} \right) + (1 - y_i) \cdot \log\left(1 - \frac{1}{1+e^{-\mathbf{w}^\top \mathbf{x}_i}} \right) \right). \tag{6.6}$$

The negative of the log-likelihood from Eq. (6.6) is sometimes referred to as cross-entropy; thus, cross-entropy minimization is equivalent to the maximum likelihood method. To make

everything more suitable for further steps, we will slightly rearrange Eq. (6.6). Notice first that

$$\left(1 - \frac{1}{1 + e^{-\mathbf{w}^\top \mathbf{x}_i}}\right) = \frac{e^{-\mathbf{w}^\top \mathbf{x}_i}}{1 + e^{-\mathbf{w}^\top \mathbf{x}_i}}$$

giving

$$\begin{aligned} ll(\mathbf{w}) &= \sum_{i=1}^{n} \Big(- y_i \cdot \log\left(1 + e^{-\mathbf{w}^\top \mathbf{x}_i}\right) + (1 - y_i) \cdot \log\left(e^{-\mathbf{w}^\top \mathbf{x}_i}\right) \\ &\qquad\qquad - (1 - y_i) \cdot \log\left(1 + e^{-\mathbf{w}^\top \mathbf{x}_i}\right) \Big) \\ &= \sum_{i=1}^{n} \left((y_i - 1)\, \mathbf{w}^\top \mathbf{x}_i + \log\left(\frac{1}{1 + e^{-\mathbf{w}^\top \mathbf{x}_i}}\right)\right). \end{aligned} \tag{6.7}$$

It does not take much effort to realize that there is no closed-form solution to $\nabla ll(\mathbf{w}) = \mathbf{0}$ (we did have this luxury in linear regression, but not here). Thus, we have to proceed with iterative optimization methods. We will calculate $\nabla ll(\mathbf{w})$ and $H_{ll(\mathbf{w})}$ to enable either method (first-order with only the gradient or second-order with the gradient and Hessian), both written as a function of inputs $\mathbf{X}$, class labels $\mathbf{y}$, and the current parameter vector. We can calculate the first and second partial derivatives of $ll(\mathbf{w})$ as follows

$$\begin{aligned} \frac{\partial ll(\mathbf{w})}{\partial w_j} &= \sum_{i=1}^{n} \left((y_i - 1) \cdot x_{ij} - \frac{1}{1 + e^{-\mathbf{w}^\top \mathbf{x}_i}} \cdot e^{-\mathbf{w}^\top \mathbf{x}_i} \cdot (-x_{ij}) \right) \\ &= \sum_{i=1}^{n} x_{ij} \cdot \left(y_i - 1 + \frac{e^{-\mathbf{w}^\top \mathbf{x}_i}}{1 + e^{\mathbf{w}^\top \mathbf{x}_i}} \right) \\ &= \sum_{i=1}^{n} x_{ij} \cdot \left(y_i - \frac{1}{1 + e^{-\mathbf{w}^\top \mathbf{x}_i}} \right) \\ &= \mathbf{f}_j^\top (\mathbf{y} - \mathbf{p}), \end{aligned}$$

where $\mathbf{f}_j$ is the j-th column (feature) of data matrix $\mathbf{X}$, $\mathbf{y}$ is an n-dimensional column vector of class labels and $\mathbf{p}$ is an n-dimensional column vector of (estimated) posterior probabilities $p_i = P(Y_i = 1 | \mathbf{x}_i, \mathbf{w})$, for $i = 1, ..., n$. Considering partial derivatives for every component of $\mathbf{w}$, we have

$$\nabla ll(\mathbf{w}) = \mathbf{X}^\top (\mathbf{y} - \mathbf{p}). \tag{6.8}$$

The second partial derivative of the log-likelihood function can be found as

$$\begin{aligned} \frac{\partial^2 ll(\mathbf{w})}{\partial w_j \partial w_d} &= \sum_{i=1}^{n} x_{ij} \cdot \frac{e^{-\mathbf{w}^\top \mathbf{x}_i}}{\left(1 + e^{-\mathbf{w}^\top \mathbf{x}_i}\right)^2} \cdot (-x_{ik}) \\ &= -\sum_{i=1}^{n} x_{ij} \cdot \frac{1}{1 + e^{-\mathbf{w}^\top \mathbf{x}_i}} \cdot \left(1 - \frac{1}{1 + e^{-\mathbf{w}^\top \mathbf{x}_i}}\right) \cdot x_{ik} \\ &= -\mathbf{f}_j^\top \mathbf{P} (\mathbf{I} - \mathbf{P}) \mathbf{f}_d, \end{aligned}$$

where $\mathbf{P}$ is an $n \times n$ diagonal matrix with $P_{ii} = p_i = P(Y_i = 1|\mathbf{x}_i, \mathbf{w})$ and $\mathbf{I}$ is an $n \times n$ identity matrix. The Hessian matrix $H_{ll(\mathbf{w})}$ can now be calculated as

$$H_{ll(\mathbf{w})} = -\mathbf{X}^\top \mathbf{P} \left(\mathbf{I} - \mathbf{P}\right) \mathbf{X}. \tag{6.9}$$

This is a negative semi-definite matrix, which guarantees that the optimum we find will be a global maximum. Negative semi-definite Hessian corresponds to a concave likelihood function and has a global maximum (unique if negative definite). Substituting Eqs. (6.8-6.9) into Newton-Raphson's method results in the following weight update rule

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} + \left(\mathbf{X}^\top \mathbf{P}^{(t)} \left(\mathbf{I} - \mathbf{P}^{(t)}\right) \mathbf{X}\right)^{-1} \mathbf{X}^\top \left(\mathbf{y} - \mathbf{p}^{(t)}\right), \tag{6.10}$$

where the initial weights $\mathbf{w}^{(0)}$ can be calculated using the ordinary least squares regression as $\mathbf{w}^{(0)} = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{y}$. Note that the second term on the right-hand side of Eq. (6.10) is calculated in each iteration t; thus we wrote $\mathbf{P}$ and $\mathbf{p}$ as $\mathbf{P}^{(t)}$ and $\mathbf{p}^{(t)}$, respectively, to indicate that $\mathbf{w}^{(t)}$ was used to calculate them.

The computational complexity of this procedure is $O(d^3+d^2n)$ in each iteration, assuming $O(d^3)$ time for finding matrix inverses. If this is infeasible for the given dataset, such as if the number of features d is large, we can use a first-order gradient descent update (which only requires $O(dn)$ to compute the matrix vector product) or quasi-Newton methods that approximate the Hessian (e.g., LBFGS).

Weighted conditional likelihood function

In certain situations, it may be justified to allow for unequal importance of each data point. This modifies the conditional likelihood function from Eq. (6.5) to

$$l(\mathbf{w}) = \prod_{i=1}^{n} p_i^{c_i y_i} \cdot (1 - p_i)^{c_i (1 - y_i)},$$

where $0 \leq c_i \leq 1$ is a cost for data point i. Taking that $\mathbf{C} = \text{diag}\left(c_1, c_2, \ldots, c_n\right)$ we can now express the gradient of the log-likelihood as

$$\nabla ll(\mathbf{w}) = \mathbf{X}^\top \mathbf{C} \left(\mathbf{y} - \mathbf{p}\right)$$

and the Hessian as

$$H_{ll(\mathbf{w})} = -\mathbf{X}^\top \mathbf{C} \mathbf{P} \left(\mathbf{I} - \mathbf{P}\right) \mathbf{X}.$$

It is interesting to observe that the Hessian remains negative semi-definite. Thus, the update rule is expected to converge to a global maximum.

6.1.3 Stochastic optimization for logistic regression

We have derived that the weight update rule depends on the data set $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ and the predictions on all training examples using the weight vector from the current step. As in Algorithm 3, we can also use stochastic gradient descent to optimize the logistic regression model. We will first rewrite the update rule of the (first-order) gradient descent method as

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} + \Delta \mathbf{w}^{(t)},$$

where

$$\begin{aligned}\Delta \mathbf{w}^{(t)} &= \eta \mathbf{X}^\top \left(\mathbf{y} - \mathbf{p}^{(t)}\right) \\ &= \eta \sum_{i=1}^{n} \mathbf{x}_i (y_i - p_i).\end{aligned}$$

We can see that the weight update is simply a linear combination of training data points. This batch gradient step is an unbiased estimate of the gradient of the true function $\int_{\mathcal{X}} \sum_{y \in \mathcal{Y}} p(\mathbf{x}, y)\mathbf{x}(y - \sigma(\mathbf{x}^\top \mathbf{w}))d\mathbf{x}dy$, because we have i.i.d. samples and so this sum converges to this integral over all possible values. Similarly, using one sample to compute the gradient is also an unbiased estimate and has been shown to converge under certain step-size conditions. When the training data is large, it may be beneficial to update the weight vector after each data point is presented to the learning algorithm, rather than computing the batch update for all samples. That is, if data point $\mathbf{x}_t$ with its class label y_t is presented to the learner, the stochastic gradient descent weight update is

$$\Delta \mathbf{w}^{(t)} = \eta \mathbf{x}_t (y_t - p_t).$$

This stochastic gradient descent is a form of stochastic approximation, which comes from a wider class of methods in the area of stochastic optimization. The batch method is often also called sample average approximation.

The training algorithm can now be revised to randomly draw one data point at a time from $\mathcal{D}$ and then update the current weights using the previous equation. Typically, in practice, this entails iterating one or more times over the dataset in order (assuming it is random, with i.i.d. samples). The conditions for convergence typically include conditions on the step-sizes, requiring them to decrease over time. As with batch gradient descent, these stochastic gradient descent updates will converge, though with more oscillation around the true weight vector, with the decreasing step-size progressively smoothing out these oscillations.

6.1.4 Issues with minimizing Euclidean distance

A natural question is why we went down this route for linear classification. Instead of explicitly assuming $P(Y = 1|\mathbf{x}, \mathbf{w})$ is a Bernoulli distribution and computing the maximum likelihood solution for $\sigma(\mathbf{x}^\top \mathbf{w}) = E[Y|\mathbf{x}] = P(Y = 1|\mathbf{x}, \mathbf{w})$, we could have simply decided to use $\sigma(\mathbf{x}^\top \mathbf{w})$ to predict targets $y \in \{0, 1\}$ and then tried to minimize their difference, using our favorite loss (the squared loss). Unfortunately, this more haphazard problem specification results in a non-convex optimization. In fact, there is a result that using the Euclidean error for the sigmoid transfer gives exponentially many local minima in the number of features [1]. For interest about this alternate route, we will show that this direction leads to a non-convex optimization.

Let the error function with Euclidean distance now be written as

$$\text{Err}(\mathbf{w}) = \sum_{i=1}^{n} (y_i - p_i)^2 \qquad \triangleright\, p_i = \sigma(\mathbf{x}_i^\top \mathbf{w}), \quad e_i = y_i - p_i$$

The minimization of $\text{Err}(\mathbf{w})$ is formally expressed as

$$\begin{aligned}\mathbf{w}^* &= \arg\min_{\mathbf{w}} \{\text{Err}(\mathbf{w})\} \\ &= \arg\min_{\mathbf{w}} \left\{ \sum_{i=1}^{n} (y_i - p_i)^2 \right\}. \end{aligned} \tag{6.11}$$

Similar to the maximum likelihood process, our goal will be to calculate the gradient vector and the Hessian of the error function. The partial derivatives of the error function can be calculated as follows

$$\begin{aligned}\frac{\partial \text{Err}(\mathbf{w})}{\partial w_j} &= \frac{\partial}{\partial w_j} \sum_{i=1}^{n} e_i^2 \\ &= \sum_{i=1}^{n} 2 \cdot e_i \cdot \frac{\partial e_i}{\partial w_j} \\ &= 2 \cdot \sum_{i=1}^{n} \left(y_i - \frac{1}{1+e^{-\mathbf{w}^\top \mathbf{x}_i}} \right) \cdot \frac{1}{(1+e^{-\mathbf{w}^\top \mathbf{x}_i})^2} \cdot e^{-\mathbf{w}^\top \mathbf{x}_i} \cdot (-x_{ij}) \\ &= -2 \cdot \sum_{i=1}^{n} x_{ij} \cdot \frac{1}{1+e^{-\mathbf{w}^\top \mathbf{x}_i}} \cdot \left(1 - \frac{1}{1+e^{-\mathbf{w}^\top \mathbf{x}_i}} \right) \cdot \left(y_i - \frac{1}{1+e^{-\mathbf{w}^\top \mathbf{x}_i}} \right) \\ &= -2\mathbf{f}_j^\top \mathbf{P} \left(\mathbf{I} - \mathbf{P} \right) \left(\mathbf{y} - \mathbf{p} \right). \end{aligned}$$

This provides the gradient vector in the following form

$$\nabla \text{Err}(\mathbf{w}) = -2\mathbf{X}^\top \mathbf{P} \left(\mathbf{I} - \mathbf{P} \right) \left(\mathbf{y} - \mathbf{p} \right).$$

Matrix $\mathbf{J} = \mathbf{P} \left(\mathbf{I} - \mathbf{P} \right) \mathbf{X}$ is referred to as Jacobian. In general, Jacobian is an $n \times d$ matrix calculated as

$$J_{\text{Err}(\mathbf{w})} = \begin{bmatrix} \frac{\partial e_1}{\partial w_1} & \frac{\partial e_1}{\partial w_2} & \cdots & \frac{\partial e_1}{\partial w_d} \\ \vdots & \ddots & & \\ & & & \\ \frac{\partial e_n}{\partial w_1} & & & \frac{\partial e_n}{\partial w_d} \end{bmatrix}.$$

The second partial derivative of the error function can be found as

$$\begin{aligned}\frac{\partial^2 \text{Err}(\mathbf{w})}{\partial w_j \partial w_d} &= 2 \cdot \sum_{i=1}^{n} \frac{\partial e_i}{\partial w_d} \cdot \frac{\partial e_i}{\partial w_j} + e_i \cdot \frac{\partial^2 e_i}{\partial w_j \partial w_d} \\ &= 2 \cdot \sum_{i=1}^{n} x_{ij} \cdot \left(p_i^2 (1-p_i)^2 + p_i \cdot (1-p_i) \cdot (2p_i - 1) \cdot (y_i - p_i) \right) \cdot x_{ik}. \end{aligned}$$

Thus, the Hessian can be computed as

$$\begin{aligned} H_{\text{Err}(\mathbf{w})} &= 2\mathbf{X}^\top \left(\mathbf{I} - \mathbf{P} \right)^\top \mathbf{P}^\top \mathbf{P} \left(\mathbf{I} - \mathbf{P} \right) \mathbf{X} + 2\mathbf{X}^\top \left(\mathbf{I} - \mathbf{P} \right)^\top \mathbf{P}^\top \mathbf{E} (2\mathbf{P} - \mathbf{I}) \mathbf{X} \\ &= 2\mathbf{J}^\top \mathbf{J} + 2\mathbf{J}^\top \mathbf{E} (2\mathbf{P} - \mathbf{I}) \mathbf{X}, \end{aligned}$$

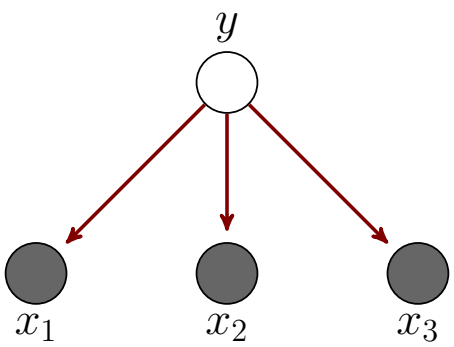


Figure 6.3: Naive Bayes graphical model, with three features.

where $\mathbf{P} = \text{diag}\{\mathbf{p}\}$, $\mathbf{E} = \text{diag}\{\mathbf{e}\}$ is a diagonal matrix containing elements $E_{ii} = e_i = y_i - p_i$ and $\mathbf{I}$ is an identity matrix.

We can now see that the Hessian is not guaranteed to be positive semi-definite. This means that $\text{Err}(\mathbf{w})$ is not convex, i.e. it must have multiple minima with different values of the objective function. Finding a global optimum depends on how favorable the initial solution $\mathbf{w}^{(0)}$ is and how well the weight update step can escape local minima to find better ones. Minimization of this non-convex function, however, will be much more problematic than the convex cross-entropy.

6.2 Naive Bayes Classifier

Naive Bayes classification is a generative approach to prediction. So far, we have discussed discriminative approaches (linear regression, logistic regression), which attempt to learn $p(y|\mathbf{x})$. For a generative setting, we learn $p(\mathbf{x}, y) = p(\mathbf{x}|y)p(y)$. As you can imagine, this can be a more difficult undertaking, as we also need to learn the distribution over the features themselves. For naive Bayes, we significantly simply learning this joint distribution by making a strong assumption: the features are conditionally independent given the label. This assumption is demonstrated by the graphical model in Figure 6.3.

As with logistic regression, even though we learn a generative model, the decision rule for labeling a point as class 1 (i.e., $y = 1$) is

$$p(y = 1|\mathbf{x}) \geq p(y = 0|\mathbf{x})$$

where now $p(y = 1|\mathbf{x}) = p(\mathbf{x}|y = 1)p(y = 1)$. To start, we will assume a simpler setting with binary features, and then address continuous features. Note that naive Bayes is a linear classifier for binary features; more generally, however, it is not necessarily a linear classifier. Note that a linear classifier is one in which the two classes are separated by a linear plane, i.e., the decision boundary is according to some linear combination of features.

6.2.1 Binary features and linear classification

Let $\mathcal{D} = \{(\mathbf{x}_i, y\}_{i=1}^n$ be an input data set, where $\mathcal{X} = \{0, 1\}^d$ and $\mathcal{Y} = \{0, 1\}$. Under the naive Bayes assumption, the features are independent given the class label. Therefore, we

can write

$$p(\mathbf{x}|y) = \prod_{i=1}^{d} p(x_i|y).$$

A suitable choice for this simpler univariate probabilities is a Bernoulli distribution, since each x_j is binary, giving

$$p(x_j|y=c) = p_{j,c}^{x_j}(1-p_{j,c})^{1-x_j}$$

The parameters for the Bernoulli distributions are $p_{j,c} = p(x_j = 1|y = c)$, with a different parameter $p_{j,c}$ for each class value c and for each feature. We can easily learn this parameter from data by calculating

$$p_{j,c} = \frac{\text{number of times } x_j = 1 \text{ for class } c}{\text{number of datapoints labeled as class } c}.$$

Similarly, we can learn the prior $p_c = p(y = c)$ using

$$p_c = p(y=c) = \frac{\text{number of datapoint labeled as class } c}{\text{total number of datapoints}}.$$

Notice that this approach could also be accomplished for more classes than just two. The prediction on a new point $\mathbf{x}$ is then

$$\begin{aligned}
\max_{c\in\mathcal{Y}} p(y=c|\mathbf{x}) &= \max_{c\in\mathcal{Y}} p(\mathbf{x}|y=c)p(y=c) \\
&= \max_{c\in\mathcal{Y}} \prod_{j=1}^{d} p(x_j|y=c)p(y=c) \\
&= \max_{c\in\mathcal{Y}} \prod_{j=1}^{d} p_{j,c}p_c
\end{aligned}$$

Exercise: The solution above is intuitive, and comes from similarly deriving the maximum likelihood solution. Assuming that you have n datapoints and the chosen distribution $p(x_i|y)$ is Bernoulli as described above, derive the maximum likelihood parameters $p_{j,c}, p_c$ for $i = 1, \ldots, d, c = 0, 1$. To make things simpler, use the log of the likelihood.

Linear classification boundary with binary features and targets

Interestingly, naive Bayes classifier with binary features and two classes is a linear classifier. This is somewhat surprising, as this generative approach looks very different from what we did before. To see why this is the case, notice that the classifier will make a positive decision when

$$p(y=1|\mathbf{x}) \geq p(y=0|\mathbf{x})$$

that is, when

$$p(\mathbf{x}|y=1)p(y=1) \geq p(\mathbf{x}|y=0)p(y=0)$$

We will shorten this notation using $p(y = 0) = p(0)$, $p(\mathbf{x}|y = 0) = p(\mathbf{x}|0)$, etc. Using the naive Bayes assumption, we now have

$$p(1) \prod_{j=1}^{d} p(x_j|1) \geq p(0) \prod_{j=1}^{d} p(x_j|0)$$

which, after applying a logarithm, then becomes

$$\log p(1) + \sum_{j=1}^{d} \log p(x_j|1) \geq \log p(0) + \sum_{j=1}^{d} \log p(x_j|0)$$

Let us now investigate class-conditional probabilities $p(x_j|y)$, when $y \in \{0, 1\}$. Recall that each feature is Bernoulli distributed, i.e.

$$p(x_j|1) = p_{j,1}^{x_j}(1 - p_{j,1})^{1-x_j}$$

and

$$p(x_j|0) = p_{j,0}^{x_j}(1 - p_{j,0})^{1-x_j}$$

where parameters $p_{j,c}$ are estimated from the training set. Taking $p(y = c) = p_c$, we have

$$\sum_{j=1}^{d} x_j \log \frac{p_{j,1}(1 - p_{j,0})}{(1 - p_{j,1})p_{j,0}} + \sum_{j=1}^{d} \log \frac{1 - p_{j,1}}{1 - p_{j,0}} + \log \frac{p_1}{p_0} \geq 0$$

We can write the previous expression as

$$w_0 + \sum_{j=1}^{d} w_j x_j \geq 0$$

where

$$w_0 = \log \frac{p_1}{p_0} + \sum_{j=1}^{d} \log \frac{1 - p_{j,1}}{1 - p_{j,0}}$$
$$w_j = \log \frac{p_{j,1}(1 - p_{j,0})}{(1 - p_{j,1})p_{j,0}} \qquad j \in \{1, 2, \ldots, d\}$$

Therefore, in the case of binary features, naive Bayes is a linear classifier.

6.2.2 Continuous naive Bayes

For continuous features, a Bernoulli distribution is no longer appropriate for $p(x_j|y)$ and we need to choose a different conditional distribution $p(\mathbf{x}|y)$. A common choice is a Gaussian distribution, now with a different mean and variance for each feature and class, $\mu_{j,c}, \sigma_{j,c}^2$:

$$p(x_j|y = c) = (2\pi\sigma_{j,c}^2)^{-1/2} \exp\left(-\frac{(x_j - \mu_{j,c})^2}{2\sigma_{j,c}^2}\right).$$

Since y is still discrete, we can approximate $p(y)$ using counts as before. The maximum likelihood mean and variance parameters correspond to the sample mean and sample covariance for each given class separately. This involves computing the mean and variance of feature j across the datapoints labeled with class c:

$$\mu_{j,c} = \frac{\sum_{i=1}^{n} 1(y_i = c)x_j}{\text{number of datapoints labeled as class } c}$$
$$\sigma^2_{j,c} = \frac{\sum_{i=1}^{n} 1(y_i = c)(x_j - \mu_{j,c})^2}{\text{number of datapoints labeled as class } c}$$

Exercise: Derive the maximum likelihood formulation for a Gaussian naive Bayes model, and check that the solution does in fact match the sample mean and variance for each feature and class separately, as above.

6.3 Multinomial logistic regression

Now let us consider discriminative multiclass classification, where $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{Y} = \{1, 2, \ldots, k\}$. This setting arises naturally in machine learning, where there is often more than two categories. For example, if we want to predict the blood type (A, B, AB and O) of an individual, then we have four classes. Here we discuss multiclass classification where we only want to label a datapoint with one class out of k. In other settings, one might want to label a datapoint with multiple classes; this is briefly mentioned at the end of this section.

We can nicely generalize to this setting using the idea of multinomials and the corresponding link function, as with the other generalized linear models. The multinomial distribution is a member of the exponential family. We can write

$$p(\mathbf{y}|\mathbf{x}) = \frac{1}{y_1! \ldots y_k!} p(y_1 = 1|\mathbf{x})^{y_1} \ldots, p(y_k = 1|\mathbf{x})^{y_k} \tag{6.12}$$

where the usual numerator $n! = 1$ because $n = \sum_{j=1}^{k} y_j = 1$ since we can only have one class value. As with logistic regression, we can parametrize $p(y_j = 1|\mathbf{x}) = \sigma(\mathbf{x}^\top \mathbf{w}_j)$. However, we must also ensure that $\sum_{j=1}^{k} p(y_j = 1|\mathbf{x}) = 1$. To do so, we "pivot" around the final class, $p(y_k = 1|\mathbf{x}) = 1 - \sum_{j=1}^{k-1} p(y_j = 1|\mathbf{x})$ and only explicitly learn $\mathbf{w}_1, \ldots, \mathbf{w}_{k-1}$. Note that these models are not learned independently, because they are tied by the probability for the last class. The parameters can be represented as a matrix $\mathbf{W} \in \mathbb{R}^{d \times k}$ where $\mathbf{W} = [\mathbf{w}_1, \ldots, \mathbf{w}_k]$ is composed of k weight vectors with $\mathbf{w}_k = \mathbf{0}$. We will see why we fix $\mathbf{w}_k = \mathbf{0}$.

The transfer (inverse of the link) for this setting is the softmax transfer

$$\begin{aligned}\text{softmax}(\mathbf{x}^\top \mathbf{W}) &= \left[\frac{\exp(\mathbf{x}^\top \mathbf{w}_1)}{\sum_{j=1}^{k} \exp(\mathbf{x}^\top \mathbf{w}_j)}, \ldots, \frac{\exp(\mathbf{x}^\top \mathbf{w}_k)}{\sum_{j=1}^{k} \exp(\mathbf{x}^\top \mathbf{w}_j)}\right] \\ &= \left[\frac{\exp(\mathbf{x}^\top \mathbf{w}_1)}{\mathbf{1}^\top \exp(\mathbf{x}^\top \mathbf{W})}, \ldots, \frac{\exp(\mathbf{x}^\top \mathbf{w}_k)}{\mathbf{1}^\top \exp(\mathbf{x}^\top \mathbf{W})}\right]\end{aligned}$$

and the prediction is $\text{softmax}(\mathbf{x}) = \hat{\mathbf{y}} \in [0, 1]^k$, which gives the probability in each entry of being labeled as that class, where $\hat{\mathbf{y}}^\top \mathbf{1} = 1$ signifying that the probabilities sum to 1. Note that this model encompasses the binary setting for logistic regression, because

$\sigma(\mathbf{x}^\top \mathbf{w}) = (1+\exp(-\mathbf{x}^\top \mathbf{w}))^{-1} = \frac{\exp(\mathbf{x}^\top \mathbf{w})}{1+\exp(\mathbf{x}^\top \mathbf{w})}$. The weights for multinomial logistic regression with two classes are then $\mathbf{W} = [\mathbf{w},\ \mathbf{0}]$ giving

$$\begin{aligned} p(y=0|\mathbf{x}) &= \frac{\exp(\mathbf{x}^\top \mathbf{w})}{\mathbf{1}^\top \exp(\mathbf{x}^\top \mathbf{W})} \\ &= \frac{\exp(\mathbf{x}^\top \mathbf{w})}{\exp(\mathbf{x}^\top \mathbf{w}) + \exp(\mathbf{x}^\top \mathbf{0})} \\ &= \frac{\exp(\mathbf{x}^\top \mathbf{w})}{\exp(\mathbf{x}^\top \mathbf{w}) + 1} \\ &= \sigma(\mathbf{x}^\top \mathbf{w}). \end{aligned}$$

Similarly, for $k > 2$, by fixing $\mathbf{w}_k = \mathbf{0}$, the other weights $\mathbf{w}_1, \ldots, \mathbf{w}_{k-1}$ are learned to ensure that $p(y=k|\mathbf{x}) = \frac{\exp(\mathbf{x}^\top \mathbf{w}_k)}{\mathbf{1}^\top \exp(\mathbf{x}^\top \mathbf{W})} = \frac{1}{1+\sum_{j=1}^{k-1} \exp(\mathbf{x}^\top \mathbf{w}_j)}$ and that $\sum_{j=1}^{k} p(y=j|\mathbf{x}) = 1$.

With the parameters of the model parameterized by $\mathbf{W}$ and the softmax transfer, we can determine the maximum likelihood formulation. By plugging in the parameterization into Equation (6.12), taking the negative log of that likelihood and dropping constants, we arrive at the following loss for samples $(\mathbf{x}_1, \mathbf{y}_1), \ldots, (\mathbf{x}_n, \mathbf{y}_n)$

$$\min_{\mathbf{W} \in \mathbb{R}^{d \times k} : \mathbf{W}_{:k} = \mathbf{0}} \sum_{i=1}^{n} \log\left(\mathbf{1}^\top \exp(\mathbf{x}_i^\top \mathbf{W})\right) - \mathbf{x}_i^\top \mathbf{W} \mathbf{y}_i$$

with gradient

$$\nabla \sum_{i=1}^{n} \left(\log\left(\mathbf{1}^\top \exp(\mathbf{x}_i^\top \mathbf{W})\right) - \mathbf{x}_i^\top \mathbf{W} \mathbf{y}_i\right) = \sum_{i=1}^{n} \frac{\exp(\mathbf{x}_i^\top \mathbf{W})^\top \mathbf{x}_i^\top}{\mathbf{1}^\top \exp(\mathbf{x}_i^\top \mathbf{W})} - \mathbf{x}_i \mathbf{y}_i^\top.$$

As before, we do not have a closed form solution for this gradient, and will use iterative methods to solve for $\mathbf{W}$. Note that here, unlike previous methods, we have a constraint on part of the variable. However, this was solely written this way for convenience. We do not optimize $\mathbf{W}_{:k}$, as it is fixed at zero; one can rewrite this minimization and gradient to only apply to the $W_{:(1:k-1)}$. This corresponds to initializing $\mathbf{W}_{:k} = \mathbf{0}$, and then only using the first $k-1$ columns of the gradient in the update to $W_{:(1:k-1)}$.

The final prediction $\text{softmax}(\mathbf{x}^\top \mathbf{W}) \in [0, 1]$ gives the probabilities of being in a class. As with logistic regression, to pick one class, the highest probability value is chosen. For example, with $k = 4$, we might predict $[0.1 \quad 0.2 \quad 0.6 \quad 0.1]$ and so decide to classify the point into class 3.

Remark about overlapping classes: If you want to predict multiple classes for a datapoint $\mathbf{x}$, then a common strategy is to learn separate binary predictors for each class. Each predictor is queried separately, and a datapoint will label each class as 0 or 1, with potentially more than one class having a 1. Above, we examined the case where the datapoint was exclusively in one of the provided classes, by setting $n = 1$ in the multinomial.

Chapter 7

Representations for machine learning

At first, it might seem that the applicability of linear regression and classification to real-life problems is greatly limited. After all, it is not clear whether it is realistic (most of the time) to assume that the target variable is a linear combination of features. Fortunately, the applicability of linear regression is broader than originally thought. The main idea is to apply a non-linear transformation to the data matrix $\mathbf{x}$ prior to the fitting step, which then enables a non-linear fit. Obtaining such a useful feature representation is a central problem in machine learning.

We will first examine fixed representations for linear regression: polynomial curve fitting and radial basis function (RBF) networks. Then, we will discuss learning representations.

7.1 Radial basis function networks and kernel representations

The idea of radial basis function (RBF) networks is a natural generalization of the polynomial curve fitting and approaches from the previous Section. Given data set $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$, we start by picking p points to serve as the "centers" in the input space $\mathcal{X}$. We denote those centers as $\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_p$. Usually, these can be selected from $\mathcal{D}$ or computed using some clustering technique (e.g. the EM algorithm, K-means).

When the clusters are determined using a Gaussian mixture model, the basis functions can be selected as

$$\phi_j(\mathbf{x}) \quad = \quad e^{-\frac{1}{2}(\mathbf{x}-\mathbf{c}_j)^T \Sigma_j^{-1} (\mathbf{x}-\mathbf{c}_j)},$$

where the cluster centers and the covariance matrix are found during clustering. When K-means or other clustering is used, we can use

$$\phi_j(\mathbf{x}) = e^{-\frac{\left\|\mathbf{x}-\mathbf{c}_j\right\|^2}{2\sigma_j^2}},$$

where σ_j's can be separately optimized; e.g. using a validation set. In the context of multidimensional transformations from $\mathbf{x}$ to $\mathbf{\Phi}$, the basis functions can also be referred to as *kernel functions*, i.e. $\phi_j(\mathbf{x}) = k_j(\mathbf{x}, \mathbf{c}_j)$. Matrix

$$\mathbf{\Phi} = \begin{bmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \cdots & \phi_p(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & & \\ \vdots & & \ddots & \\ \phi_0(\mathbf{x}_n) & & & \phi_p(\mathbf{x}_n) \end{bmatrix}$$

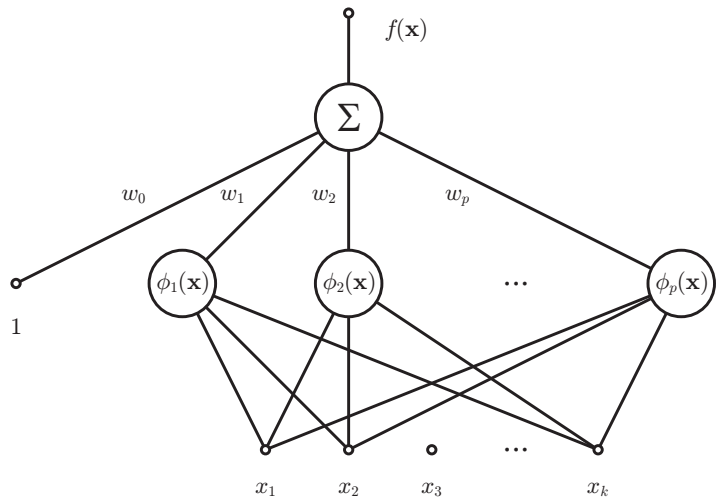


Figure 7.1: Radial basis function network.

is now used as a new data matrix. For a given input $\mathbf{x}$, the prediction of the target y will be calculated as

$$\begin{aligned} f(\mathbf{x}) &= w_0 + \sum_{j=1}^{p} w_j \phi_j(\mathbf{x}) \\ &= \sum_{j=0}^{p} w_j \phi_j(\mathbf{x}) \end{aligned}$$

where $\phi_0(\mathbf{x}) = 1$ and $\mathbf{w}$ is to be found. It can be proved that with a sufficiently large number of radial basis functions we can accurately approximate any function. As seen in Figure 7.1, we can think of RBFs as neural networks.

RBF networks and kernel representations are highly related. The main distinction is that kernel representations use any kernel function for the similarity measure $k(\mathbf{x}, \mathbf{c}_j) = \phi_j(\mathbf{x})$, where radial basis functions are one example of a kernel. In addition, if an RBF kernel is chosen, for kernel representations typical the centers are selected from the training dataset. For RBF networks, the selection of the centers is left generally as an important step, where they can be selected from the training set but can also be selected in other ways.

7.2 Learning representations

There are many approaches to learning representations. Two dominant approaches are (semi-supervised) matrix factorization techniques and neural networks. Neural networks build on the generalized linear models we have discussed, stacking multiple generalized linear models together. Matrix factorization techniques (e.g., dimensionality reduction, sparse coding) typically factorize the input data into a dictionary and a new representation (a basis). We will first discuss neural networks, and then discuss the many unsupervised and semisupervised learning techniques that are encompassed by matrix factorizations.

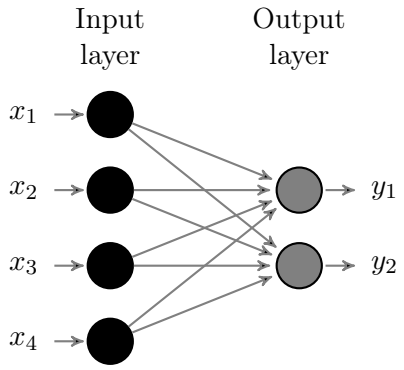


Figure 7.2: Generalized linear model, such as logistic regression.

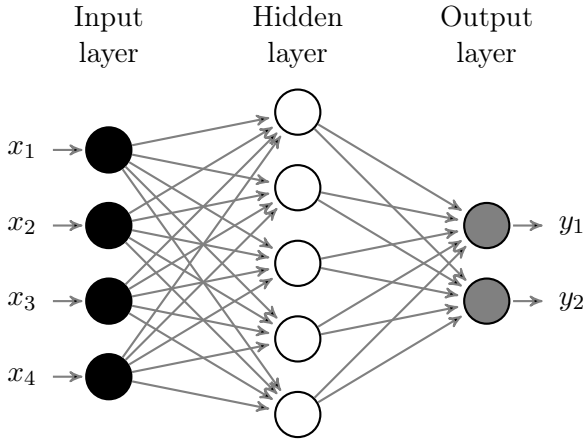


Figure 7.3: Standard two-layer neural network.

7.2.1 Neural networks

Neural networks are a form of supervised representation learning. As before, the goal is to learn a function of inputs, f, to produce a prediction of the target: $f(\mathbf{x})$. The addition of hidden layers, with non-linear activation functions, enables learning of nonlinear functions f. For some intuition, one can consider that all the first hidden layers constitute representation layer, with learning on the last layer corresponding to supervised prediction part. Figure 7.2 shows the graphical model for the generalized linear models we discussed in the previous chapters, where the weights and corresponding transfer can be thought of as being on the arrows (as they are not random variables). Figure 7.3 shows a neural network with one hidden-layer; this is called a two-layer neural network, as there are two layers of weights.

In the figure, the neural network inputs a 4-dimensional feature vector $\mathbf{x} = [x_1,\ x_2,\ x_3,\ x_4]$ (i.e., $d = 4$) and outputs a 2-dimensional prediction $\mathbf{y} = [y_1,\ y_2]$ (i.e., $m = 2$). The hidden layer consists of a mapping from $\mathbf{x}$ to a new representation that is 5-dimensional (i.e., $k_1 = 5$ as per the notation below). For the neural network, let each node in this hidden representation be indexed by $k \in \{1, \ldots, 5\}$. Each h_k consists of a transformation of a linear weighting of $\mathbf{x}$, such as a sigmoid transfer: $h_k = \sigma\left(\sum_{j=1}^{d} x_j w_{kj}\right) = \sigma\left(\mathbf{x}\mathbf{w}_k\right)$ where $\mathbf{w}_k \in \mathbb{R}^d$ is the weights on the first layer used to produce the kth node in the hidden representation.

Example 15: For a simple example, consider $d = 1$ (i.e., one input observation), $m = 1$ (i.e., one output), $k_1 = 2$ (i.e., 2-dimensional hidden layer) and a sigmoid transfer to get the first hidden layer. Assume we are given one instance (x, y). Then input observation x is transformed into

$$\mathbf{h} = [h_1,\ h_2], \qquad \text{with } h_1 = \sigma(x w_1^{(2)}) \text{ and } h_2 = \sigma(x w_2^{(2)}) \qquad \text{for } w_1^{(2)}, w_2^{(2)} \in \mathbb{R}.$$

To avoid transpose notation, we used $\mathbf{x} \in \mathbb{R}^{1\times d}$ to give one row of the data matrix $\mathbf{X} \in \mathbb{R}^{n\times d}$, and row vector $\mathbf{h} \in \mathbb{R}^{1\times k_1}$. We use the superscript notation to distinguish between the weights in the first and last layer. It may seem counter-intuitive why we label $\mathbf{w}^{(2)}$ for the input layer, and $\mathbf{w}^{(1)}$ for the output layer, but you will see below it makes notation simpler to start indexing from the output layer.

Once we have $\mathbf{h}$, we can pretend that $\mathbf{h}$ is the new input representation and go ahead and learn a (generalized) linear model on this last layer. Let's consider two cases: $y \in \mathbb{R}$

and $y \in \{0, 1\}$. If $y \in \mathbb{R}$, we use linear regression for this last layer and so learn weights $\mathbf{w}^{(2)} \in \mathbb{R}^2$ such that $\mathbf{h}\mathbf{w}^{(2)}$ approximates the true output y. If $y \in \{0, 1\}$, we use logistic regression for this last layer and so learn weights $\mathbf{w}^{(2)} \in \mathbb{R}^2$ such that $\sigma(\mathbf{h}\mathbf{w}^{(2)})$ approximates the true output y. □

Now we consider the more general case with any d, k_1, m. To provide some intuition for this more general setting, we will begin with one hidden layer, for the sigmoid transfer function and cross-entropy output loss. For logistic regression we estimated $\mathbf{W} \in \mathbb{R}^{d \times m}$, with $f(\mathbf{x}\mathbf{W}) = \sigma(\mathbf{x}\mathbf{W}) \approx \mathbf{y}$. We will predict an output vector $\mathbf{y} \in \mathbb{R}^m$, because it will make later generalizations more clear-cut and make notation for the weights in each layer more uniform. When we add a hidden layer, we have two parameter matrices $\mathbf{W}^{(2)} \in \mathbb{R}^{d \times k_1}$ and $\mathbf{W}^{(1)} \in \mathbb{R}^{k_1 \times m}$, where k_1 is the dimension of the hidden layer

$$\mathbf{h} = \sigma(\mathbf{W}^{(2)}\mathbf{x}) = \begin{bmatrix} \sigma(\mathbf{x}\mathbf{W}^{(2)}_{:1}) \\ \sigma(\mathbf{x}\mathbf{W}^{(2)}_{:2}) \\ \vdots \\ \sigma(\mathbf{x}\mathbf{W}^{(2)}_{:k_1}) \end{bmatrix} \in \mathbb{R}^{k_1}$$

where the sigmoid function is applied to each entry in $\mathbf{x}\mathbf{W}^{(2)}$ and $\mathbf{h}\mathbf{W}^{(1)}$. This hidden layer is the new set of features and again you will do the regular logistic regression optimization to learn weights on $\mathbf{h}$:

$$p(y = 1|\mathbf{x}) = \sigma(\mathbf{h}\mathbf{W}^{(1)}) = \sigma(\sigma(\mathbf{x}\mathbf{W}^{(2)})\mathbf{W}^{(1)}).$$

With the probabilistic model and parameter specified, we now need to derive an algorithm to obtain those parameters. As before, we take a maximum likelihood approach and derive gradient descent updates. This composition of transfers seems to complicate matters, but we can still take the gradient w.r.t. our parameters. We simply have more parameters now: $\mathbf{W}^{(2)} \in \mathbb{R}^{k_1 \times d}, \mathbf{W}^{(1)} \in \mathbb{R}^{1 \times k_1}$. Once we have the gradient w.r.t. each parameter matrix, we simply take a step in the direction of the negative of the gradient, as usual. The gradients for these parameters share information; for computational efficiency, the gradient is computed first for $\mathbf{W}^{(1)}$, and duplicate gradient information sent back to compute the gradient for $\mathbf{W}^{(2)}$. This algorithm is typically called *back propagation*, which we describe next.

In general, we can compute the gradient for any number of hidden layers. Denote each differentiable transfer function $f_1, \ldots, f_H$, ordered with f_1 as the output transfer, and $k_1, \ldots, k_{H-1}$ as the hidden dimensions with $H - 1$ hidden layers. Then the output from the neural network is

$$f_1\left(f_2\left(\ldots f_{H-1}\left(f_H\left(\mathbf{x}\mathbf{W}^{(H)}\right)\mathbf{W}^{(H-1)}\right)\ldots\right)\mathbf{W}^{(1)}\right)$$

where $\mathbf{W}^{(1)} \in \mathbb{R}^{k_1 \times m}$, $\mathbf{W}^{(2)} \in \mathbb{R}^{k_2 \times k_1}$, $\ldots, \mathbf{W}^{(H)} \in \mathbb{R}^{d \times k_{H-1}}$.

Backpropagation algorithm

We will start by deriving back propagation for two layers; the extension to multiple layers will be more clear given this derivation. Due to the size of the network, we will often learn

with stochastic gradient descent. Therefore, we will first compute this gradient assuming we only have one sample $(\mathbf{x}, \mathbf{y})$.

The back-propagation algorithm is simply gradient descent on a non-convex objective, with a careful ordering of computation to avoid repeating computation. In particular, one first propagates forward and computes variable $\mathbf{h} = f_2(\mathbf{x}\mathbf{W}^{(2)}) \in \mathbb{R}^{1\times k}$ and then $\hat{\mathbf{y}} = f_1(f_2(\mathbf{x}\mathbf{W}^{(2)})\mathbf{W}^{(1)}) = f_1(\mathbf{h}\mathbf{W}^{(1)})$. We then compute the error between our prediction $\hat{\mathbf{y}}$ and the true label. We take the gradient of this error (loss) w.r.t. to our parameters; in this case, for efficient computation, the best ordering is to compute the gradient w.r.t. to the last parameter $\mathbf{W}^{(1)}$ first, and then $\mathbf{W}^{(2)}$. This is the reason for the term back-propagation, since the error is propagated backward from the last layer first.

The choices then involve picking the transfers at each layer, the number of hidden nodes and the loss for the last layer. The matching convex loss $L(\cdot, y)$ depends on the chosen $p(y|\mathbf{x})$ and corresponding transfer function for the last layer of the neural network, just as with generalized linear models. For ease of notation, we define this error function as

$$\text{Err}(\mathbf{W}^{(1)}, \mathbf{W}^{(2)}) = \sum_{k=1}^{m} L(f_1(f_2(\mathbf{x}\mathbf{W}^{(2)})\mathbf{W}^{(1)}_{:k}), \mathbf{y}_k)$$

for one sample $(\mathbf{x}, \mathbf{y})$. For example, for $p(y = 1|\mathbf{x})$ Gaussian and identity transfer f_2, we get $\text{Err}(\mathbf{W}^{(1)}, \mathbf{W}^{(2)}) = (f_2(\mathbf{x}\mathbf{W}^{(2)})\mathbf{W}^{(1)} - y)^2$. If $p(y = 1|\mathbf{x})$ is a Bernoulli distribution, then we would chose the logistic regression loss (the cross entropy).

As before, we will compute gradients of the loss w.r.t. our parameters. First, we take the partial derivative w.r.t. the parameters $\mathbf{W}^{(1)}$ (assuming $\mathbf{W}^{(2)}$ is fixed).

$$\begin{aligned}
\frac{\partial \text{Err}(\mathbf{W}^{(1)}, \mathbf{W}^{(2)})}{\partial \mathbf{W}^{(1)}_{jk}} &= \frac{\partial L(f_1(f_2(\mathbf{x}\mathbf{W}^{(2)})\mathbf{W}^{(1)}), \mathbf{y})}{\partial \mathbf{W}^{(1)}_{jk}} \\
&= \left(\frac{\partial L(\hat{\mathbf{y}}_k, \mathbf{y}_k)}{\partial \hat{\mathbf{y}}_k}\right) \frac{\partial \hat{\mathbf{y}}_k}{\partial \mathbf{W}^{(1)}_{jk}} \qquad \triangleright\, \hat{\mathbf{y}}_k = f_1(\mathbf{h}\mathbf{W}^{(1)}_{:k})
\end{aligned}$$

where only $\hat{\mathbf{y}}_k$ is affected by $\mathbf{W}^{(1)}_{jk}$ in the loss, and so the gradient for the others is zero. Continuing,

$$\begin{aligned}
\frac{\partial \text{Err}(\mathbf{W}^{(1)}, \mathbf{W}^{(2)})}{\partial \mathbf{W}^{(1)}_{jk}} &= \left(\frac{\partial L(\hat{\mathbf{y}}_k, \mathbf{y}_k)}{\partial \hat{\mathbf{y}}_k}\right) \frac{\partial f_1(\boldsymbol{\theta}^{(1)}_k)}{\partial \boldsymbol{\theta}^{(1)}_k} \frac{\partial \boldsymbol{\theta}^{(1)}_k}{\partial \mathbf{W}^{(1)}_{jk}} \qquad \triangleright\, \boldsymbol{\theta}^{(1)}_k = \mathbf{h}\mathbf{W}^{(1)}_{:k} \\
&= \left(\frac{\partial L(\hat{\mathbf{y}}_k, \mathbf{y}_k)}{\partial \hat{\mathbf{y}}_k}\right) \frac{\partial f_1(\boldsymbol{\theta}^{(1)}_k)}{\partial \boldsymbol{\theta}^{(1)}_k} \mathbf{h}_j
\end{aligned}$$

At this point these equations are abstract; but they are simple to compute for the losses and transfers we have examined. For example, for $L(\hat{\mathbf{y}}_k, \mathbf{y}_k) = \frac{1}{2}(\hat{\mathbf{y}}_k - \mathbf{y}_k)^2$, and f_2 the identity, we get

$$\begin{aligned}
\frac{\partial L(\hat{\mathbf{y}}_k, \mathbf{y}_k)}{\partial \hat{\mathbf{y}}_k} &= (\hat{\mathbf{y}}_k - \mathbf{y}_k) \\
\frac{\partial f_1(\boldsymbol{\theta}^{(1)}_k)}{\partial \boldsymbol{\theta}^{(1)}_k} &= 1
\end{aligned}$$

giving

$$\frac{\partial \text{Err}(\mathbf{W}^{(1)}, \mathbf{W}^{(2)})}{\partial \mathbf{W}^{(1)}_{jk}} = \left(\frac{\partial L(\hat{\mathbf{y}}_k, \mathbf{y}_k)}{\partial \hat{\mathbf{y}}_k}\right) \frac{\partial f_1(\boldsymbol{\theta}^{(1)}_k)}{\partial \boldsymbol{\theta}^{(1)}_k} \mathbf{h}_j = (\hat{\mathbf{y}}_k - \mathbf{y}_k)\mathbf{h}_j.$$

The gradient update is as usual with $\mathbf{W}^{(1)} = \mathbf{W}^{(1)} - \alpha(\hat{\mathbf{y}} - \mathbf{y})\mathbf{h}^\top$ for some step-size α.

Next, we compute the partial gradient with respect to $\mathbf{W}^{(2)}$. Now, however, the entire output variable $\mathbf{y} \in \mathbb{R}^{1\times m}$ is affect by the choice of $\mathbf{W}^{(2)}_{ij}$ for all $i \in \{1, \ldots, k_2\}$, $j \in \{1, \ldots, k_1\}$. Therefore, we need to take the partial derivative w.r.t. all of $\mathbf{y}$.

$$\begin{aligned}
\frac{\partial \text{Err}(\mathbf{W}^{(1)}, \mathbf{W}^{(2)})}{\partial \mathbf{W}^{(2)}_{ij}} &= \frac{\partial \sum_{k=1}^m L(f_1(f_2(\mathbf{x}\mathbf{W}^{(2)})\mathbf{W}^{(1)}_{:k}), \mathbf{y}_k)}{\partial \mathbf{W}^{(2)}_{ij}} \\
&= \sum_{k=1}^m \frac{\partial L(\hat{\mathbf{y}}_k, \mathbf{y}_k)}{\partial \hat{\mathbf{y}}_k} \frac{\partial \hat{\mathbf{y}}_k}{\partial \mathbf{W}^{(2)}_{ij}} && \triangleright\ \hat{\mathbf{y}}_k = f_1(\mathbf{h}\mathbf{W}^{(1)}_{:k}) = f_1(\boldsymbol{\theta}^{(1)}_k) \\
&= \sum_{k=1}^m \frac{\partial L(\hat{\mathbf{y}}_k, \mathbf{y}_k)}{\partial \hat{\mathbf{y}}_k} \frac{\partial f_1(\boldsymbol{\theta}^{(1)}_k)}{\partial \boldsymbol{\theta}^{(1)}_k} \frac{\partial \boldsymbol{\theta}^{(1)}_k}{\partial \mathbf{W}^{(2)}_{ij}}.
\end{aligned}$$

Continuing,

$$\begin{aligned}
\frac{\partial \boldsymbol{\theta}^{(1)}_k}{\partial \mathbf{W}^{(2)}_{ij}} = \frac{\partial \mathbf{h}\mathbf{W}^{(1)}_{:k}}{\partial \mathbf{W}^{(2)}_{ij}} &= \frac{\partial \sum_{l=1}^k \mathbf{h}_l \mathbf{W}^{(1)}_{lk}}{\partial \mathbf{W}^{(2)}_{ij}} \\
&= \frac{\partial \sum_{l=1}^k f_2(\mathbf{x}\mathbf{W}^{(2)}_{:l})\mathbf{W}^{(1)}_{lk}}{\partial \mathbf{W}^{(2)}_{ij}} \\
&= \sum_{l=1}^k \mathbf{W}^{(1)}_{lk} \frac{\partial f_2(\mathbf{x}\mathbf{W}^{(2)}_{:l})}{\partial \mathbf{W}^{(2)}_{ij}} \\
&= \mathbf{W}^{(1)}_{jk} \frac{\partial f_2(\mathbf{x}\mathbf{W}^{(2)}_{:j})}{\partial \mathbf{W}^{(2)}_{ij}}
\end{aligned}$$

because $\frac{\partial f_2(\mathbf{x}\mathbf{W}^{(2)}_{:l})}{\partial \mathbf{W}^{(2)}_{ij}} = 0$ for $l \neq j$. Now continuing the chain rule

$$\begin{aligned}
\frac{\partial f_2(\mathbf{x}\mathbf{W}^{(2)}_{:j})}{\partial \mathbf{W}^{(2)}_{ij}} &= \frac{\partial f_2(\boldsymbol{\theta}^{(2)}_j)}{\partial \boldsymbol{\theta}^{(2)}_j} \frac{\partial \boldsymbol{\theta}^{(2)}_j}{\partial \mathbf{W}^{(2)}_{ij}} && \triangleright\ \boldsymbol{\theta}^{(2)}_j = \mathbf{x}\mathbf{W}^{(2)}_{:j} \\
&= \frac{\partial f_2(\boldsymbol{\theta}^{(2)}_j)}{\partial \boldsymbol{\theta}^{(2)}_j} \mathbf{x}_i.
\end{aligned}$$

Putting this back together, we get

$$\begin{aligned}
\frac{\partial \text{Err}(\mathbf{W}^{(1)}, \mathbf{W}^{(2)})}{\partial \mathbf{W}^{(2)}_{ij}} &= \sum_{k=1}^m \frac{\partial L(\hat{\mathbf{y}}_k, \mathbf{y}_k)}{\partial \hat{\mathbf{y}}_k} \frac{\partial f_1(\boldsymbol{\theta}^{(1)}_k)}{\partial \boldsymbol{\theta}^{(1)}_k} \frac{\partial \boldsymbol{\theta}^{(1)}_k}{\partial \mathbf{W}^{(2)}_{ij}} \\
&= \sum_{k=1}^m \frac{\partial L(\hat{\mathbf{y}}_k, \mathbf{y}_k)}{\partial \hat{\mathbf{y}}_k} \frac{\partial f_1(\boldsymbol{\theta}^{(1)}_k)}{\partial \boldsymbol{\theta}^{(1)}_k} \mathbf{W}^{(1)}_{jk} \frac{\partial f_2(\boldsymbol{\theta}^{(2)}_j)}{\partial \boldsymbol{\theta}^{(2)}_j} \mathbf{x}_i.
\end{aligned}$$

Notice that some of gradient is the same as for $\mathbf{W}^{(1)}$, i.e.

$$\boldsymbol{\delta}_k^{(1)} = \frac{\partial L(\hat{\mathbf{y}}_k, \mathbf{y}_k)}{\partial \hat{\mathbf{y}}_k} \frac{\partial f_1(\boldsymbol{\theta}_k^{(1)})}{\partial \boldsymbol{\theta}_k^{(1)}}$$

Computing these components only needs to be done once for $\mathbf{W}^{(1)}$, and this information propagated back to get the gradient for $\mathbf{W}^{(2)}$. The difference is in the gradient $\frac{\partial \boldsymbol{\theta}^{(1)}}{\partial \mathbf{W}^{(2)}}$, because $\mathbf{h}$ relies on $\mathbf{W}^{(2)}$. For $\mathbf{W}^{(1)}$, $\mathbf{h} = f_2(\mathbf{x}_i \mathbf{W}^{(2)})$ is a constant, and so does not affect the gradient for $\mathbf{W}^{(1)}$. The final gradient is

$$\begin{aligned}
\frac{\partial \text{Err}(\mathbf{W}^{(1)}, \mathbf{W}^{(2)})}{\partial \mathbf{W}_{ij}^{(2)}} &= \left(\sum_{k=1}^{m} \boldsymbol{\delta}_k^{(1)} \mathbf{W}_{jk}^{(1)} \right) \frac{\partial f_2(\boldsymbol{\theta}_j^{(2)})}{\partial \boldsymbol{\theta}_j^{(2)}} \mathbf{x}_i \\
&= \left(\mathbf{W}_{j:}^{(1)} \boldsymbol{\delta}^{(1)} \right) \frac{\partial f_2(\boldsymbol{\theta}_j^{(2)})}{\partial \boldsymbol{\theta}_j^{(2)}} \mathbf{x}_i
\end{aligned}$$

If another layer is added before $\mathbf{W}^{(2)}$, then the information propagated backward is

$$\boldsymbol{\delta}_j^{(2)} = \left(\mathbf{W}_{j:}^{(1)} \boldsymbol{\delta}^{(1)} \right) \frac{\partial f_2(\boldsymbol{\theta}_j^{(2)})}{\partial \boldsymbol{\theta}_j^{(2)}}$$

and $\mathbf{x}_i$ is replaced with $\mathbf{h}_i^{(2)}$. The gradient for $\mathbf{W}_{ij}^{(3)}$ is

$$\left(\mathbf{W}_{j:}^{(2)} \boldsymbol{\delta}^{(2)} \right) \frac{\partial f_3(\boldsymbol{\theta}_j^{(3)})}{\partial \boldsymbol{\theta}_j^{(3)}} \mathbf{x}_i$$

Example 16: Let $p(y = 1|\mathbf{x})$ be a Bernoulli distribution, with f_1 and f_2 both sigmoid functions. The loss is the cross-entropy. We can derive the two-layer update rule with these settings, by plugging-in above.

$$\begin{aligned}
L(\hat{y}, y) &= -y \log(\hat{y}) - (1 - y) \log(1 - \hat{y}) && \triangleright \text{ cross-entropy} \\
\frac{\partial L(\hat{y}, y)}{\partial \hat{y}} &= -\frac{y}{\hat{y}} + \frac{1 - y}{1 - \hat{y}} \\
f_2(\mathbf{x}\mathbf{W}_{:j}^{(2)}) &= \sigma(\mathbf{x}\mathbf{W}_{:j}^{(2)}) = \frac{1}{1 + \exp(-\mathbf{x}\mathbf{W}_{:j}^{(2)})} \\
f_1(\mathbf{h}\mathbf{W}_{:k}^{(1)}) &= \sigma(\mathbf{h}\mathbf{W}_{:k}^{(1)}) = \frac{1}{1 + \exp(-\mathbf{h}\mathbf{W}_{:k}^{(1)})} \\
\partial \sigma(\theta) &= \sigma(\theta)(1 - \sigma(\theta))
\end{aligned}$$

Now we can compute the backpropagation update by first propagating forward

$$\begin{aligned}
\mathbf{h} &= \sigma(\mathbf{x}\mathbf{W}^{(2)}) \\
\hat{\mathbf{y}} &= \sigma(\mathbf{h}\mathbf{W}^{(1)})
\end{aligned}$$

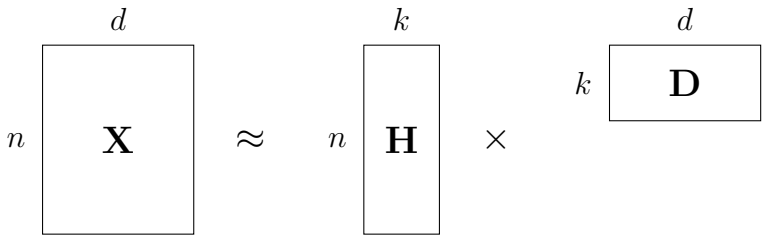


Figure 7.4: Matrix factorization of data matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$.

and then propagating the gradient back

$$\begin{aligned}
\boldsymbol{\delta}_k^{(1)} &= \frac{\partial L(\hat{\mathbf{y}}_k, \mathbf{y}_k)}{\partial \hat{\mathbf{y}}_k} \frac{\partial f_1(\boldsymbol{\theta}_k^{(1)})}{\partial \boldsymbol{\theta}_k^{(1)}} \\
&= \left(-\frac{\mathbf{y}_k}{\hat{\mathbf{y}}_k} + \frac{1 - \mathbf{y}_k}{1 - \hat{\mathbf{y}}_k} \right) \hat{\mathbf{y}}_k (1 - \hat{\mathbf{y}}_k) \\
&= -\mathbf{y}_k (1 - \hat{\mathbf{y}}_k) + (1 - \mathbf{y}_k) \hat{\mathbf{y}}_k \\
\frac{\partial}{\partial \mathbf{W}_{jk}^{(1)}} &= \boldsymbol{\delta}_k^{(1)} \mathbf{h}_j \\
\boldsymbol{\delta}_j^{(2)} &= \left(\mathbf{W}_{j:}^{(1)} \boldsymbol{\delta}^{(1)} \right) \mathbf{h}_j (1 - \mathbf{h}_j) \\
\frac{\partial}{\partial \mathbf{W}_{ij}^{(2)}} &= \boldsymbol{\delta}_j^{(2)} \mathbf{x}_i
\end{aligned}$$

The update simply consists of stepping in the direction of these gradients, as is usual for gradient descent. We start with some initial $\mathbf{W}^{(1)}$ and $\mathbf{W}^{(2)}$ (say filled with random values), and then apply the gradient descent rules with these gradients. □

7.2.2 Unsupervised learning and matrix factorization

Another strategy to obtaining a new representation is through matrix factorization. The data matrix $\mathbf{X}$ is factorized into a dictionary $\mathbf{D}$ and a basis or new representation $\mathbf{H}$ (see Figure 7.4). In fact, many unsupervised learning algorithms (e.g., dimensionality reduction, sparse coding) and semi-supervised learning algorithms (e.g., supervised dictionary learning) can actually be formulated as matrix factorizations. We will look at k-means clustering and principal components analysis as an example. The remaining algorithms are simply summarized in the below table. This general approach to obtaining a new representation using factorization is called **dictionary learning**.

K-means clustering is an unsupervised learning problem to group data points into k clusters by minimizing distances to the mean of each cluster. This problem is not usually thought of as a representation learning approach, because the cluster number is not typically used as a representation. However, we nonetheless start with k-means because it is an intuitive example of how these unsupervised learning algorithms can be thought of as matrix factorization. Further, the clustering approach can be seen as a representation learning

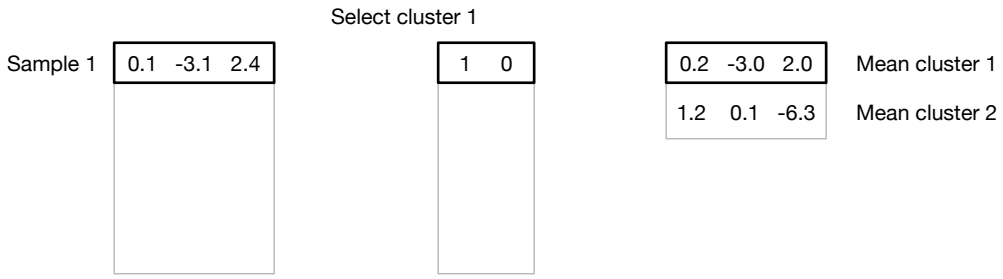


Figure 7.5: K-means clustering as a matrix factorization for data matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$.

approach, because it is a learned discretization of the space. We will discuss this view of k-means after discussing it as a matrix factorization.

Imagine that you have two clusters ($k = 2$), with data dimension $d = 3$. Let $\mathbf{d}_1$ be the mean for cluster 1 and $\mathbf{d}_2$ the mean for cluster 2. The goal is to minimize the squared ℓ_2 distance of each data point $\mathbf{x}$ to its cluster center

$$\|\mathbf{x} - \sum_{i=1}^{2} 1\left(\mathbf{x} \text{ in cluster } i\right) \mathbf{d}_i\|_2^2 = \|\mathbf{x} - \mathbf{h}\mathbf{D}\|_2^2$$

where $\mathbf{h} = [1 \quad 0]$ or $\mathbf{h} = [0 \quad 1]$ and $\mathbf{D} = [\mathbf{d}_1 \; ; \; \mathbf{d}_2]$. An example is depicted in Figure 7.5. For a point $\mathbf{x} = [0.1 \quad -3.1 \quad 2.4]$, $\mathbf{h} = [1 \quad 0]$, meaning it is placed in cluster 1 with mean $\mathbf{d}_1 = [0.2 \quad -3.0 \quad 2.0]$. It would incur more error to place $\mathbf{x}$ in cluster 2 which has a mean that is more dissimilar: $\mathbf{d}_2 = [1.2 \quad 0.1 \quad -6.3]$.

The overall minimization is defined across all the samples, giving loss

$$\min_{\substack{\mathbf{H} \in \{0,1\}^{n \times k}, \mathbf{1}\mathbf{H} = \mathbf{1} \\ \mathbf{D} \in \mathbb{R}^{k \times d}}} \|\mathbf{X} - \mathbf{H}\mathbf{D}\|_F^2.$$

Different clusters vectors $\mathbf{h}$ are learned for each $\mathbf{x}$, but the dictionary of means is shared amongst all the data points. The specified optimization should pick dictionary $\mathbf{D}$ of means that provides the smallest distances to points in the training dataset.

Principal components analysis (PCA) is a standard dimensionality reduction technique, where the input data $\mathbf{x} \in \mathbb{R}^{1 \times d}$ is projected into a lower dimensional $\mathbf{h} \in \mathbb{R}^{1 \times k}$ spanned by the space of principal components. These principal components are the directions of maximal variance in the data. To obtain these k principal components $\mathbf{D} \in \mathbb{R}^{k \times d}$, the common solution technique is to obtain the singular value decomposition of the data matrix $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top \in \mathbb{R}^{n \times d}$, giving

$$\mathbf{D} = \mathbf{V}_k^\top \in \mathbb{R}^{k \times d}$$
$$\mathbf{H} = \mathbf{U}_k \mathbf{\Sigma}_k \in \mathbb{R}^{n \times k}$$

where $\mathbf{\Sigma}_k \in \mathbb{R}^{k \times k}$ consists of the top largest k singular values (in descending order) and $\mathbf{U}_k \in \mathbb{R}^{n \times k}$ and $\mathbf{V}_k \in \mathbb{R}^{k \times d}$ are the corresponding singular vectors, i.e., $\mathbf{U}_k = \mathbf{U}_{:,1:k}$ and $\mathbf{V}_k = \mathbf{V}_{:,1:k}$. The new representation for $\mathbf{X}$ (using PCA) is this $\mathbf{H}$. Note that PCA does

not subselect features, but rather creates new features: The generated $\mathbf{h}$ is not a subset of the original $\mathbf{x}$.

This dimensionality reduction technique can also be formulated as a matrix factorization. The corresponding optimization has been shown to be

$$\min_{\mathbf{D}\in\mathbb{R}^{k\times d},\mathbf{H}\in\mathbb{R}^{n\times k}} \|\mathbf{X}-\mathbf{H}\mathbf{D}\|_F^2$$

One simple way to see why is to recall the well-known Eckart-Young-Mirsky theorem that the rank k matrix $\hat{\mathbf{X}}$ that best approximates $\mathbf{X}$, in terms of minimal Frobenius norm, is $\hat{\mathbf{X}} = \mathbf{U}_k\mathbf{\Sigma}_k\mathbf{V}_k^\top$.

As with k-means clustering, it may be hard to immediately see why $\mathbf{h}$ generated by PCA could be useful as a representation. In fact, PCA is often used for visualization, and so is not always used for representation learning. For visualization, the projection is often aggressive to two or three dimensions. In general, however, the projection to lower dimensions has the property that it removes noise and maintains only the most meaningful directions. This projection, therefore, helps speed learning by reducing the number of features and promoting generalization, by preventing overfitting to the noise.

Sparse coding takes a different approach, where the input data is expanded into a sparse representation. Sparse coding is biologically motivated [12], based on sparse activations for memory in the mammalian brain. Another interpretation is that sparse coding effectively discretizes the space, like k-means clustering, but with overlapping clusters and an associated magnitude of how much a point belongs to that cluster.

A common strategy to obtain sparse representations is to use a sparse regularizer on the learned representation $\mathbf{h}$. This corresponds to the optimization

$$\min_{\mathbf{D}\in\mathbb{R}^{k\times d},\mathbf{H}\in\mathbb{R}^{n\times k}} \|\mathbf{X}-\mathbf{H}\mathbf{D}\|_F^2 + \lambda\sum_{i=1}^{k}\|\mathbf{H}_{:i}\|_1 + \lambda\sum_{i=1}^{k}\|\mathbf{D}_{i:}\|_2^2$$

As discussed in Section 4.4.2, the ℓ_1 regularizer promotes zeroed entries, and so prefers $\mathbf{H}$ with as many zeros as possible. A regularizer is also added to $\mathbf{D}$, to ensure that $\mathbf{D}$ does not become too large; otherwise, all the weight in $\mathbf{D}\mathbf{H}$ would be shifted to $\mathbf{D}$. As an exercise, see if you can explain why, and what this means for identifiability.

In general, there are many variants of unsupervised learning algorithms that actually correspond to factorizing the data matrix; additional details are given in Appendix D. We additionally give details on how to learn these factorizations in the appendix. As with previous algorithms, they are simply gradient descent on the (matrix) variables. The only distinction here is that it is common to use block coordinate descent, instead of the more standard gradient descent algorithm. This distinction is minor, and it would be perfectly valid to use standard gradient descent.

Chapter 8

Evaluation of Learning Algorithms

The majority of this book has focused on algorithm derivation and obtaining models, but we have yet to address how to evaluate these models. The maximum likelihood formalism for deriving learning algorithms provides some consistency results, where in the limit of samples we can discuss the convergence point of an estimator. In practice, however, we would like to evaluate the algorithms based on a finite sample. Imagine a setting where you learn two models, say using logistic regression with two different regularization parameters. Which of these two models is "better"? What does it even mean to say better? Do you want to say the model is better for this problem (data setting), or across multiple problems? Are we trying to compare algorithms or models obtained from a specific instance of an algorithm? How can we be confident that the measured performance accurately reflects the performance we expect to see on new data? These questions are largely separate from our previous questions of effectively optimizing a specified objective, and rather starts to ask questions about the properties of that objective and about empirical properties of learned models.

In this chapter, we provide theoretical and empirical tools to better evaluate the properties of learning algorithms. We begin with some basic finite-sample theoretical results, that relate the complexity of the model class to the number of samples required to obtain a reasonable estimate of expected error (generalization error). This section will also introduce the ideas of optimizing over a function class, and our goals for obtaining the best model in terms of generalization error. The area dealing with these types of theoretical characterizations is called *statistical learning theory*. We will discuss one result using *concentration inequalities* and *Rademacher complexity* to characterize model-class complexity; for further information, you could consider this tutorial on the topic [6].

Then, we will discuss how to compare algorithms empirically. In most real-world settings, you will choose between algorithms based on their performance on available data. You want this choice to be reflective of how well those algorithms will perform on new data. Towards this goal, we will discuss how to split data and how to use statistical significance tests to provide some level of confidence that one algorithm or model is better than another, under some specific criteria. We will rarely be able to make strong conclusions based on experiments, but we can build up some evidence on the algorithm properties.

These tools are arguably the most critical aspects of properly using machine learning algorithms in practice. One can learn a complex model, but without any understanding of how it is expected to perform in practice on new data, it is not viable to actual use these models. Whether an algorithm is used for scientific purposes or deployed in real systems, have an understanding of its properties both theoretically and empirically is key to obtain expected outcomes. This chapter only begins to scratch the surface of these tools, with the goal to pique your interest and direct you towards more material for learning about evaluation.

8.1 A brief introduction to generalization bounds

Our goal throughout this book has been to obtain a function, based on a set of examples, that predicts accurately: produces low expected error across the space of possible examples. We cannot, however, measure the expected error. Statistically, we know that with a sufficient sample, we can approximate an expectation. Here, we quantify this more carefully for learned functions.

Our goal more precisely is to select a function from a function class $\mathcal{H}$ to minimize a loss function $\ell : \mathbb{R} \times \mathbb{R} \to [0, \infty)$ in expectation over all pairs $(\mathbf{x}, y)$

$$\min_{f \in \mathcal{H}} \mathbb{E}[\ell(f(\boldsymbol{X}), Y)].$$

For example, in linear regression, $\mathcal{H} = \{f : \mathbb{R}^d \to \mathbb{R} \mid f(\mathbf{x}) = \mathbf{x}^\top \mathbf{w}, \text{ for any } \mathbf{w} \in \mathbb{R}^d\}$. This space of functions $\mathcal{H}$ represents all possible linear functions of inputs $\mathbf{x} \in \mathbb{R}^d$, to produce a scalar output. Our goal in linear regression was to minimize a proxy to the true expected error, i.e., the sample error: $\frac{1}{n}\sum_{i=1}^n \ell(f(\mathbf{x}_i), y_i)$. Now a natural question to ask is: does this sample error provide an accurate estimate of the true expected error? And what does it tell us about the true generalization performance, i.e., true expected error?

Let's start with a simple example, using linear regression. Assume a bounded function class $\mathcal{H}$, where $\mathcal{H} = \{f : \mathbb{R}^d \to \mathbb{R} \mid f(\mathbf{x}) = \mathbf{x}^\top \mathbf{w}, \text{ for any } \mathbf{w} \in \mathbb{R}^d \text{ such that } \|\mathbf{w}\|_2 \leq B_w\}$ for some finite scalar $B_w > 0$. Assume the input features come from a bounded space, such that for all $\mathbf{x}$, $\|\mathbf{x}\|_2 \leq B_x$ for some finite scalar $B_x > 0$. Then for approximate error

$$\widehat{\text{Err}}(f) = \frac{1}{n}\sum_{i=1}^n \ell(f(\mathbf{x}_i), y_i)$$

and true error

$$\text{Err}(f) = \mathbb{E}[\ell(f(\boldsymbol{X}), Y)] = \int_{\mathcal{X}\times\mathcal{Y}} p(\mathbf{x}, y)\ell(f(\mathbf{x}), y)d\mathbf{x}dy$$

we get that with probability $1 - \delta$, for $\delta \in (0, 1]$,

$$\text{Err}(f) \leq \widehat{\text{Err}}(f) + \frac{B_x B_w}{\sqrt{n}} + \sqrt{\frac{\ln(1/\delta)}{n}}. \tag{8.1}$$

With increasing samples n, the second two terms disappear and the sample error approaches the true expected error. This bound show the rate at which this discrepancy disappears. For a higher confidence—small δ making $\ln(1/\delta)$ larger—more samples are need for the third term to be small. This third term is obtained using *concentration inequalities*, which enable us to state the rate at which a sample mean gets close to its expected value. For possibly large values of features or learned weights, the second term can be big and can again require the more samples. The second term reflects the properties of our function class: a simpler class, with small bounded weights, can have a more accurate estimate of the loss on a smaller number of samples. More generally, this complexity measure is called the *Rademacher complexity*[1], where, for the linear functions we considered, this complexity is bounded by $\frac{B_x B_w}{\sqrt{n}}$.

We will now build up to a generalization result, similar to (8.1), but for more general functions.

[1]If you have heard of VC dimension, we will discuss the connection between Rademacher and VC dimension below. They both play a role in identifying the complexity of a function class.

8.1.1 Concentration inequalities

We will examine the use of concentration inequalities with one common example: Hoeffding's inequality. For the generalization bound below, a generalization is used, called McDiarmid's inequality.

For i.i.d. random variables $X_1, \ldots, X_n$, such that $0 \leq X_i \leq 1$, let $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$ be the sample average. Then Hoeffding's inequality states that for any ϵ

$$\Pr(\bar{X} - \mathbb{E}[\bar{X}] \geq \epsilon) \leq \exp(-2n\epsilon^2).$$

We start by setting this probability value to δ, so that we can say with probability δ, $\Pr(\bar{X} - \mathbb{E}[\bar{X}] \geq \text{function}(\delta))$. We can solve for ϵ in terms of δ, to get

$$\delta = \exp(-2n\epsilon^2) \qquad \implies \epsilon = \pm\sqrt{\frac{\ln(1/\delta)}{2n}}.$$

We can either set ϵ to $\sqrt{\frac{\ln(1/\delta)}{2n}}$ or $-\sqrt{\frac{\ln(1/\delta)}{2n}}$, to bound $\bar{X}$ to be near $\mathbb{E}[\bar{X}]$ from both above and below. We get that with probability $1-\delta$, $\left|\bar{X} - \mathbb{E}[\bar{X}]\right| \leq |\epsilon| = \sqrt{\frac{\ln(1/\delta)}{2n}}$.

This concentration inequality makes few assumptions about the random variables, and does not require any distributional assumptions. Consequently, the rate of convergence to the true mean is only $1/\sqrt{n}$. Faster rates can be obtained with more assumptions.

8.1.2 Complexity of a function class

Rademacher complexity of a function class characterizes the overfitting ability of functions, on a particular sample. Function class that are typically more complex are more likely to be able to fit random noise, and so have higher Rademacher complexity. The empirical Rademacher complexity, for a sample $\{\mathbf{z}_1, \ldots, \mathbf{z}_n\}$ —where typically we consider $\mathbf{z}_i = (\mathbf{x}_i, y_i)$ — is defined as[2]

$$\hat{R}_n(\mathcal{H}) = \mathbb{E}\left[\max_{f \in \mathcal{H}} \frac{1}{n}\sum_{i=1}^{n} \sigma_i f(\mathbf{z}_i)\right]$$

where the expectation is over i.i.d. random variables $\sigma_1, \ldots, \sigma_n$ chosen uniformly from $\{-1, 1\}$. This choice reflects how well the function class can correlate with this random noise. Consider for example if $f(\mathbf{x})$ predicts 1 or -1, as in binary classification. If there exists a function in the class of functions that can perfectly match the sign of the randomly sampled σ_i, then that function produces the highest value $\sum_{i=1}^{n} \sigma_i f(\mathbf{x}_i)$. The empirical Rademacher complexity for a function class is high, if for any randomly sampled σ_i, there exists such a function within the function class (can be a different function for each $\sigma_1, \ldots, \sigma_n$). The Rademacher complexity is the expected empirical Rademacher complexity, over all possibly samples of n instances.

For function classes with high Rademacher complexity, error on the training set is unlikely to be reflective of the generalization error, until there is a sufficient number of samples. This is reflected in the generalization bound in Section 8.1.3.

[2]Here we are being a bit loose and using maximum instead of supremum, to avoid burdening the reader with new terminology. We usually deal with function classes $\mathcal{H}$ where using the supremum is equivalent to using the maximum. The supremum is used when a set does not contain a maximal point (e.g., $[0, 1)$), where the supremum provides the closest upper bound (e.g., 1 for $[0, 1)$).

Connection to VC dimension: The complexity of a function class can also be characterized by the VC dimension. The idea of VC dimension to characterize the number of points that can be separated (or shattered) by a function class. Simple functions have low VC dimension, because they are not complex enough to separate many points. More complex functions, that enable complex boundaries, have higher VC dimension. For example, for functions of the form $f((x_1, x_2)) = \text{sign}(x_1 w_1 + x_2 w_2 + w_0)$, the VC dimension is 3; more generally, for $\mathbf{x} \in \mathbb{R}^d$, the VC dimension is $d + 1$. VC dimension is a similar idea to Rademacher complexity, but it is restricted to binary classifiers. For this reason, we directly discuss the Rademacher complexity, which for binary classifiers can be bounded in terms of the VC dimension. By Sauer's Lemma, we can typically bound the Rademacher complexity of a hypothesis class by $\sqrt{\frac{2\text{VC-dimension} \ln n}{n}}$.

8.1.3 Generalization bounds

The generalization bound for a class of models can be obtained by combining the concentration inequalities to bound deviation from the mean for fewer samples, and using the Rademacher complexity to bound the difference between the sample error and true expected error across all functions in the function class. We additionally need to restrict the set of losses. We assume that the losses are Lipschitz with constant c, meaning that they do not change too quickly in a region, with c indicating the rate of change. Further, we also assume that the loss is bounded by b, i.e., attains values in $[-b, b]$. As above, if $\{\mathbf{z}_1, \ldots, \mathbf{z}_n\}$ is i.i.d., then with probability $1 - \delta$, for every $f \in \mathcal{H}$,

$$\mathbb{E}[\ell(f(\boldsymbol{X}), Y)] \leq \frac{1}{n} \sum_{i=1}^{n} \ell(f(\mathbf{x}_i), y_i) + 2cR_n(\mathcal{H}) + b\sqrt{\frac{\ln(1/\delta)}{2n}}$$

For a more precise theorem statement and a proof, see [3, Theorem 7] and [9, Theorem 1].

8.2 Comparison of Learning Algorithms

To empirically evaluate algorithms, we can consider a setting with one or more algorithms on one or more datasets. Depending on the setting, different evaluations will be employed. For a nice overview of evaluation for machine learning algorithms, see [8].

For now, let's start with a simple case, where we compare two algorithms and use the binomial test. Suppose we have a set of learning problems $\mathcal{D}_1, \mathcal{D}_2, \ldots \mathcal{D}_m$ and wish to compare learning algorithms a_1 and a_2. We can carry out such a comparison using a counting test as follows: for each data set both algorithms are evaluated in terms of the chosen performance measure and the algorithm with a higher performance accuracy is awarded a win, while the other one is given a loss (in case of exactly the same performance, we can provide a win/loss randomly).

We are now interested in providing statistical evidence that say algorithm a_1 is better than algorithm a_2. Suppose a_1 has k wins out of m and algorithm a_2 has $m - k$ wins, as shown in Table 8.1. We would like to evaluate the null hypothesis H_0 that algorithms a_1 and a_2 have the same performance by providing an alternative hypothesis H_1 that algorithm

	$\mathcal{D}_1$	$\mathcal{D}_2$	$\mathcal{D}_3$	$\mathcal{D}_4$		$\mathcal{D}_{m-1}$	$\mathcal{D}_m$
a_1	1	0	1	1	$\cdots$	0	1
a_2	0	1	0	0		1	0

Table 8.1: A counting test where learning algorithms a_1 and a_2 are compared on a set of m independent data sets. An algorithm with a better performance on a particular data set collects a win (1), whereas the other algorithm collects a loss (0).

a_1 is better than a_2. In short,

$$H_0\text{: quality}(a_1) = \text{quality}(a_2)$$
$$H_1\text{: quality}(a_1) > \text{quality}(a_2)$$

If the null hypothesis is true, the win/loss on each data set will be equally likely and determined by minor variation. Therefore, the probability of a win on any data set will be roughly equal to $p = 1/2$. Now, we can express the probability that algorithm a_1 collected k wins or more under the null hypothesis using binomial distribution

$$P = \sum_{i=k}^{m} \binom{m}{i} p^i (1-p)^{m-i}$$

and refer to it as the P-value. This value is the probability of k wins, plus the probability of $k+1$ wins, up to the probability of m wins, under the null hypothesis. A typical approach in these cases is to establish a significance value, say, $\alpha = 0.05$ and reject the null hypothesis if $P \leq \alpha$. If the P-value is greater than α we say that there is insufficient evidence for rejecting H_0. For sufficiently low P-values, we may conclude that there is sufficient evidence that algorithm a_1 is better than algorithm a_2.

The choice of the significance threshold α is somewhat arbitrary. Typically, 5% is a reasonable value, but lower values indicate that the particular situation of k wins out of m was so unlikely, that we can consider the evidence for rejecting H_0 very strong. Being able to reject the null hypothesis provides some confidence that the result did not occur by chance.

More generally, we can consider other statistical significance tests based on the distributions of the performance measures. In the above example, a binomial distribution was appropriate. If instead we considered the actual errors on the datasets, then we have pairs of real values. In this case, a common choice is the paired t-test, if both errors appear to be distributed normally and if they have similar variance. The paired t-test takes in the sampled differences between the algorithms (line 3 in Table 8.2), $d_1, \ldots, d_m$. Because again our null hypothesis is that the algorithms perform equally, under the null hypothesis the mean of these differences is 0. If the differences are normally distributed, then for the sample average $\bar{d} = \frac{1}{m}\sum_{i=1}^{m} d_i$ and sample standard deviation $S_d = \sqrt{\frac{1}{m-1}\sum_{i=1}^{m}(d_i - \bar{d})^2}$, the random variable $t = \frac{\bar{d}-0}{S_d/\sqrt{m}}$ is distributed according to the Student's t-distribution. The Student's t-distribution is approximately like a normal distribution, with a degrees-of-freedom parameter m that makes the distribution look more like a normal distribution as m becomes larger. We can now ask about the probability of this random variable T,

relative to the computed statistic. If we only care about knowing if algorithm 1 is better than algorithm 2, we conduct a one-tailed test. If the probability that T is larger than t, i.e., $p = Pr(T > t)$, is small, then we obtain some evidence that algorithm 1 is better than algorithm 2. To test if algorithm 1 is better than algorithm 2, we can swap the order of the difference; if $p = Pr(T > -t)$ is small, then we obtain some evidence that algorithm 2 is better than algorithm 1. These are both one-tailed tests, reflecting the probabilities at one end of the tails of the distribution. A two-tailed test instead asks if the two algorithms are different; in this case, one would use $p = Pr(T > |t|)$.

	$\mathcal{D}_1$	$\mathcal{D}_2$	$\mathcal{D}_3$	$\mathcal{D}_4$		$\mathcal{D}_{m-1}$	$\mathcal{D}_m$
a_1	0.11	0.08	0.15	0.12	$\cdots$	0.07	0.09
a_2	0.10	0.09	0.11	0.12	$\cdots$	0.10	0.09
d	0.01	-0.01	0.04	0.0	$\cdots$	-0.03	0.0

Table 8.2: A table of errors for two learning algorithms a_1 and a_2 are compared on a set of m independent data sets. The last row contains the differences, which are used for the paired t-test.

If the paired samples are not normally distributed, other tests are more suitable. Further, there are some tests that do not make distributional assumptions, and rather are non-parametric. For a nice summary of which test to use for different conditions, see [8, Section 6.3]

8.3 Obtaining samples of error

A key step in comparing algorithms is to obtain valid measures of performance for the comparison. So far, we have assumed that these are given. One approach to obtain unbiased samples of the error is to keep a hold-out test set. Imagine m samples are set in reserve, on which the algorithms are not trained and which we cannot look at until we are ready to evaluate. We can train two models on the training set, and then obtain m paired samples of error. We can then use the paired t-test to make claims about if the two models are statistically significantly different for the problem.

However, there are two key disadvantages to using a hold-out test set. First, usually we want to use all the data for training. Unless there is more data than can be used, keeping a hold-out test set is typically not practical. Even in this age of huge datasets, we still typically want to learn on as much (quality) data as possible. Second, once this hold-out test set has been used for evaluation, we cannot use it again because it will not provide an unbiased estimate of the expected error. For example, after getting performance of your models on that test set, one could go back and adjust meta-parameters such as the regularization parameters. However, once you have done this, the test-set has influenced the learned models and is likely to produce an optimistic estimate of performance on new data. Therefore, this hold-out test-set can only be used once.

An alternative approach to obtain estimates of error is to use resampling techniques from the whole dataset. Two common resampling techniques are k-fold cross-validation and bootstrap resampling. In the first, the data is partitioned into k disjoint sets (folds). The

model is trained on $k-1$ of the folds, and tested on the other fold; this is repeated k times where each fold acts as the test fold. This approach simulates the common learning setting where the training and test sets are disjoint. The resulting k performance estimates are mostly independent, with some dependency introduced due to dependencies between the training sets across the k runs. There is some additional bias introduced from the fact that we do not run the model on the entire training set, but rather get an estimate of the error for the algorithm trained on $n-(n/k)$. For any final models that will be put into production after performing these evaluations, we will likely train on the entire set of n instances.

The bootstrap resample treats the data uses the idea behind bootstrapping: the data constitutes a reasonable model of the data. By sampling from the data, it is like sampling from the distribution that generated the data. To generate training/test splits, the data is sampled with replacement to create the training set, and the remaining unused samples used for test. If k resamples are obtained, we again get k performance measures and can obtain a sample average of performance across different splits and use statistical significance test.

To better understand the properties of these two approaches, see the thorough and accessible explanation in [7, Chapter 5].

8.4 Performance measures for Classification Models

In classification, there are a variety of performance measures to reflect the relative importance of incorrect predictions for either class. For example, it can be more detrimental to predict a patient is not sick if they are actually sick (False Negative), resulting in a decision not to run further diagnostics and so causing serious complications from not treating the illness. When training and evaluating classification algorithms, these preferences need to be encoded. Table 8.3 summarizes some of the terminology for discussing performance of classification models.

Name	Symbol	Definition
Classification error	$error$	$error = \frac{fp+fn}{tp+fp+tn+fn}$
Classification accuracy	$accuracy$	$accuracy = 1 - error$
True positive rate	tpr	$tpr = \frac{tp}{tp+fn}$
False negative rate	fnr	$fnr = \frac{fn}{tp+fn}$
True negative rate	tnr	$tnr = \frac{tn}{tn+fp}$
False positive rate	fpr	$fpr = \frac{fp}{tn+fp}$
Precision	pr	$pr = \frac{tp}{tp+fp}$
Recall	rc	$rc = \frac{tp}{tp+fn}$

Table 8.3: Some classification measures.

Chapter 9

Advanced topics

9.1 Bayesian estimation

Maximum a posteriori and maximum likelihood approaches report the solution that corresponds to the mode of the posterior distribution and the likelihood function, respectively. This approach, however, does not consider the possibility of skewed distributions, multimodal distributions or simply large regions with similar values of $p(M|\mathcal{D})$. Bayesian estimation addresses those concerns.

The main idea in Bayesian statistics is minimization of the *posterior risk*

$$R = \int_{\mathcal{M}} \ell(M, \hat{M}) \cdot p(M|\mathcal{D}) dM$$

where $\hat{M}$ is our estimate and $\ell(M, \hat{M})$ is some loss function between two models. When $\ell(M, \hat{M}) = (M - \hat{M})^2$ (ignore the abuse of notation), we can minimize the posterior risk as follows

$$\begin{aligned} \frac{\partial}{\partial \hat{M}} R &= 2\hat{M} - 2 \int_{\mathcal{M}} M \cdot p(M|\mathcal{D}) dM \\ &= 0 \end{aligned}$$

from which it can be derived that the minimizer of the posterior risk is the posterior mean function, i.e.

$$\begin{aligned} M_B &= \int_{\mathcal{M}} M \cdot p(M|\mathcal{D}) dM \\ &= E_M[M|\mathcal{D}]. \end{aligned}$$

We shall refer to M_B as the Bayes estimator. It is important to mention that computing the posterior mean usually involves solving complex integrals. In some situations, these integrals can be solved analytically; in others, numerical integration is necessary.

Example 11. Let $\mathcal{D} = \{2, 5, 9, 5, 4, 8\}$ yet again be an i.i.d. sample from Poisson(λ_t). Suppose the prior knowledge about the parameter of the exponential distribution can be expressed using a gamma distribution with parameters $k = 3$ and $\theta = 1$. Find the Bayesian estimate of λ_t.

We want to find $E[\lambda|\mathcal{D}]$. Let us first write the posterior distribution as

$$
\begin{aligned}
p(\lambda|\mathcal{D}) &= \frac{p(\mathcal{D}|\lambda)p(\lambda)}{p(\mathcal{D})} \\
&= \frac{p(\mathcal{D}|\lambda)p(\lambda)}{\int_0^\infty p(\mathcal{D}|\lambda)p(\lambda)d\lambda},
\end{aligned}
$$

where, as shown in previous examples, we have that

$$
p(\mathcal{D}|\lambda) = \frac{\lambda^{\sum_{i=1}^n x_i} \cdot e^{-n\lambda}}{\prod_{i=1}^n x_i!}
$$

and

$$
p(\lambda) = \frac{\lambda^{k-1} e^{-\frac{\lambda}{\theta}}}{\theta^k \Gamma(k)}.
$$

Before calculating $p(\mathcal{D})$, let us first note that

$$
\int_0^\infty x^{\alpha-1} e^{-\beta x} dx = \frac{\Gamma(\alpha)}{\beta^\alpha}.
$$

Now, we can derive that

$$
\begin{aligned}
p(\mathcal{D}) &= \int_0^\infty p(\mathcal{D}|\lambda)p(\lambda)d\lambda \\
&= \int_0^\infty \frac{\lambda^{\sum_{i=1}^n x_i} \cdot e^{-n\lambda}}{\prod_{i=1}^n x_i!} \cdot \frac{\lambda^{k-1} e^{-\frac{\lambda}{\theta}}}{\theta^k \Gamma(k)} d\lambda \\
&= \frac{\Gamma(k + \sum_{i=1}^n x_i)}{\theta^k \Gamma(k) \prod_{i=1}^n x_i! (n + \frac{1}{\theta})^{\sum_{i=1}^n x_i + k}}
\end{aligned}
$$

and subsequently that

$$
\begin{aligned}
p(\lambda|\mathcal{D}) &= \frac{p(\mathcal{D}|\lambda)p(\lambda)}{p(\mathcal{D})} \\
&= \frac{\lambda^{\sum_{i=1}^n x_i} \cdot e^{-n\lambda}}{\prod_{i=1}^n x_i!} \cdot \frac{\lambda^{k-1} e^{-\frac{\lambda}{\theta}}}{\theta^k \Gamma(k)} \cdot \frac{\theta^k \Gamma(k) \prod_{i=1}^n x_i! (n + \frac{1}{\theta})^{\sum_{i=1}^n x_i + k}}{\Gamma(k + \sum_{i=1}^n x_i)} \\
&= \frac{\lambda^{k-1+\sum_{i=1}^n x_i} \cdot e^{-\lambda(n+1/\theta)} \cdot (n + \frac{1}{\theta})^{\sum_{i=1}^n x_i + k}}{\Gamma(k + \sum_{i=1}^n x_i)}.
\end{aligned}
$$

Finally,

$$
\begin{aligned}
E[\lambda|\mathcal{D}] &= \int_0^\infty \lambda p(\lambda|\mathcal{D}) d\lambda \\
&= \frac{k + \sum_{i=1}^n x_i}{n + \frac{1}{\theta}} \\
&= 5.14
\end{aligned}
$$

which is nearly the same solution as the MAP estimate found in Example 9. □

It is evident from the previous example that selection of the prior distribution has important implications on calculation of the posterior mean. We have not picked the gamma distribution by chance; that is, when the likelihood was multiplied by the prior, the resulting distribution remained in the same class of functions as the likelihood. We shall refer to such prior distributions as *conjugate priors*. Conjugate priors are also simplifying the mathematics; in fact, this is a major reason for their consideration. Interestingly, in addition to the Poisson distribution, the gamma distribution is a conjugate prior to the exponential distribution as well as the gamma distribution itself.

9.2 Parameter estimation for mixtures of distributions

We now investigate parameter estimation for mixture models, which is most commonly carried out using the *expectation-maximization (EM) algorithm*. As before, we are given a set of i.i.d. observations $\mathcal{D} = \{x_i\}_{i=1}^n$, with the goal of estimating the parameters of the mixture distribution

$$p(x|\theta) = \sum_{j=1}^{m} w_j p(x|\theta_j).$$

In the equation above, we used $\theta = (w_1, w_2, \ldots, w_m, \theta_1, \theta_2, \ldots, \theta_m)$ to combine all parameters. Just to be more concrete, we shall assume that each $p(x_i|\theta_j)$ is an exponential distribution with parameter λ_j, i.e. $p(x|\theta_j) = \lambda_j e^{-\lambda_j x}$, where $\lambda_j > 0$. Finally, we shall assume that m is given and will address simultaneous estimation of θ and m later.

Let us attempt to find the maximum likelihood solution first. By plugging the formula for $p(x|\theta)$ into the likelihood function we obtain

$$\begin{aligned} p(\mathcal{D}|\theta) &= \prod_{i=1}^{n} p(x_i|\theta) \\ &= \prod_{i=1}^{n} \left(\sum_{j=1}^{m} w_j p(x_i|\theta_j) \right), \end{aligned} \tag{9.1}$$

which, unfortunately, is difficult to maximize using differential calculus (why?). Note that although $p(\mathcal{D}|\theta)$ has $O(m^n)$ terms, it can be calculated in $O(mn)$ time as a log-likelihood.

Before introducing the EM algorithm, let us for a moment present two hypothetical scenarios that will help us to understand the algorithm. First, suppose that information is available as to which mixing component generated which data point. That is, suppose that $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$ is an i.i.d. sample from some distribution $p_{XY}(x, y)$, where $y \in \mathcal{Y} = \{1, 2, \ldots, m\}$ specifies the mixing component. How would the maximization be performed then? Let us write the likelihood function as

$$
\begin{aligned}
p(\mathcal{D}|\theta) &= \prod_{i=1}^{n} p(x_i, y_i|\theta) \\
&= \prod_{i=1}^{n} p(x_i|y_i, \theta) p(y_i|\theta) \\
&= \prod_{i=1}^{n} w_{y_i} p(x_i|\theta_{y_i}), \qquad (9.2)
\end{aligned}
$$

where $w_j = p_Y(j) = P(Y = j)$. The log-likelihood is

$$
\begin{aligned}
\log p(\mathcal{D}|\theta) &= \sum_{i=1}^{n} (\log w_{y_i} + \log p(x_i|\theta_{y_i})) \\
&= \sum_{j=1}^{m} n_j \log w_j + \sum_{i=1}^{n} \log p(x_i|\theta_{y_i}),
\end{aligned}
$$

where n_j is the number of data points in $\mathcal{D}$ generated by the j-th mixing component.

It is useful to observe here that when $\mathbf{y} = (y_1, y_2, \ldots, y_n)$ is known, the internal summation operator in Eq. (9.1) disappears. More importantly, it follows that Eq. (9.2) can be maximized in a relatively straightforward manner. Let us show how. To find $\mathbf{w} = (w_1, w_2, \ldots, w_m)$ we need to solve a constrained optimization problem, which we will do by using the method of Lagrange multipliers. We shall first form the Lagrangian function as

$$
L(\mathbf{w}, \alpha) = \sum_{j=1}^{m} n_j \log w_j + \alpha \left(\sum_{j=1}^{m} w_j - 1 \right)
$$

where α is the Lagrange multiplier. Then, by setting $\frac{\partial}{\partial w_k} L(\mathbf{w}, \alpha) = 0$ for every $k \in \mathcal{Y}$ and $\frac{\partial}{\partial \alpha} L(\mathbf{w}, \alpha) = 0$, we derive that $w_k = -\frac{n_k}{\alpha}$ and $\alpha = -n$. Thus,

$$
w_k = \frac{1}{n} \sum_{i=1}^{n} I(y_i = k),
$$

where $I(\cdot)$ is the indicator function. To find all θ_j, we recall that we assumed a mixture of exponential distributions. Thus, we proceed by setting

$$
\frac{\partial}{\partial \lambda_k} \sum_{i=1}^{n} \log p(x_i|\lambda_{y_i}) = 0,
$$

for each $k \in \mathcal{Y}$. We obtain that

$$
\lambda_k = \frac{n_k}{\sum_{i=1}^{n} I(y_i = k) \cdot x_i},
$$

which is simply the inverse mean over those data points generated by the k-th mixture component. In summary, we observe that if the mixing component designations $\mathbf{y}$ are

known, the parameter estimation is greatly simplified. This was achieved by decoupling the estimation of mixing proportions and all parameters of the mixing distributions.

In the second hypothetical scenario, suppose that parameters θ are known, and that we would like to estimate the best configuration of the mixture designations $\mathbf{y}$ (one may be tempted to call them "class labels"). This task looks like clustering in which cluster memberships need to be determined based on the known set of mixing distributions and mixing probabilities. To do this we can calculate the posterior distribution of $\mathbf{y}$ as

$$\begin{aligned} p(\mathbf{y}|\mathcal{D},\theta) &= \prod_{i=1}^{n} p(y_i|x_i,\theta) \\ &= \prod_{i=1}^{n} \frac{w_{y_i} p(x_i|\theta_{y_i})}{\sum_{j=1}^{m} w_j p(x_i|\theta_j)} \end{aligned} \tag{9.3}$$

and subsequently find the best configuration out of m^n possibilities. Obviously, because of the i.i.d. assumption each element y_i can be estimated separately and, thus, this estimation can be completed in $O(mn)$ time. The MAP estimate for y_i can be found as

$$\hat{y}_i = \arg\max_{y_i \in \mathcal{Y}} \left\{ \frac{w_{y_i} p(x_i|\theta_{y_i})}{\sum_{j=1}^{m} w_j p(x_i|\theta_j)} \right\}$$

for each $i \in \{1, 2, \ldots, n\}$.

In reality, neither "class labels" $\mathbf{y}$ nor the parameters θ are known. Fortunately, we have just seen that the optimization step is relatively straightforward if one of them is known. Therefore, the intuition behind the EM algorithm is to form an iterative procedure by *assuming* that either $\mathbf{y}$ or θ is known and calculate the other. For example, we can initially pick some value for θ, say $\theta^{(0)}$, and then estimate $\mathbf{y}$ by computing $p(\mathbf{y}|\mathcal{D},\theta^{(0)})$ as in Eq. (9.3). We can refer to this estimate as $\mathbf{y}^{(0)}$. Using $\mathbf{y}^{(0)}$ we can now refine the estimate of θ to $\theta^{(1)}$ using Eq. (9.2). We can then iterate these two steps until convergence. In the case of mixture of exponential distributions, we arrive at the following algorithm:

1. Initialize $\lambda_k^{(0)}$ and $w_k^{(0)}$ for $\forall k \in \mathcal{Y}$
2. Calculate $y_i^{(0)} = \arg\max_{k \in \mathcal{Y}} \left\{ \frac{w_k^{(0)} p(x_i|\lambda_k^{(0)})}{\sum_{j=1}^{m} w_j^{(0)} p(x_i|\lambda_j^{(0)})} \right\}$ for $\forall i \in \{1, 2, \ldots, n\}$
3. Set $t = 0$
4. Repeat until convergence
   (a) $w_k^{(t+1)} = \frac{1}{n} \sum_{i=1}^{n} I(y_i^{(t)} = j)$
   (b) $\lambda_k^{(t+1)} = \frac{\sum_{i=1}^{n} I(y_i^{(t)}=k)}{\sum_{i=1}^{n} I(y_i^{(t)}=k) \cdot x_i}$
   (c) $t = t + 1$
   (d) $y_i^{(t+1)} = \arg\max_{k \in \mathcal{Y}} \left\{ \frac{w_k^{(t)} p(x_i|\lambda_k^{(t)})}{\sum_{j=1}^{m} w_j^{(t)} p(x_i|\lambda_j^{(t)})} \right\}$
5. Report $\lambda_k^{(t)}$ and $w_k^{(t)}$ for $\forall k \in \mathcal{Y}$

This procedure is not quite yet the EM algorithm; rather, it is a version of it referred to as *classification EM algorithm*. In the next section we will introduce the EM algorithm.

The expectation-maximization algorithm

The previous procedure was designed to iteratively estimate class memberships and parameters of the distribution. In reality, it is not necessary to compute $\mathbf{y}$; after all, we only need to estimate θ. To accomplish this, at each step t, we can use $p(\mathbf{y}|\mathcal{D}, \theta^{(t)})$ to maximize the *expected log-likelihood* of both $\mathcal{D}$ and $\mathbf{y}$

$$E_{\mathbf{Y}}[\log p(\mathcal{D}, \mathbf{y}|\theta)|\theta^{(t)}] = \sum_{\mathbf{y}} \log p(\mathcal{D}, \mathbf{y}|\theta) p(\mathbf{y}|\mathcal{D}, \theta^{(t)}), \tag{9.4}$$

which can be carried out by integrating the log-likelihood function of $\mathcal{D}$ and $\mathbf{y}$ over the posterior distribution for $\mathbf{y}$ in which the current values of the parameters $\theta^{(t)}$ are assumbed to be known. We can now formulate the expression for the parameters in step $t+1$ as

$$\theta^{(t+1)} = \arg\max_{\theta} \left\{ E[\log p(\mathcal{D}, \mathbf{y}|\theta)|\theta^{(t)}] \right\}. \tag{9.5}$$

The formula above is all that is necessary to create the update rule for the EM algorithm. Note, however, that inside of it we always have to re-compute $E_{\mathbf{Y}}[\log p(\mathcal{D}, \mathbf{y}|\theta)|\theta^{(t)}]$ function because the parameters $\theta^{(t)}$ have been updated from the previous step. We then can perform maximization. Hence the name "expectation-maximization", although it is perfectly valid to think of the EM algorithm as an interative maximization of expectation from Eq. (9.4), i.e. "expectation maximization".

We now proceed as follows

$$\begin{aligned}
E[\log p(\mathcal{D}, \mathbf{y}|\theta)|\theta^{(t)}] &= \sum_{y_1=1}^{m} \cdots \sum_{y_n=1}^{m} \log p(\mathcal{D}, \mathbf{y}|\theta) p(\mathbf{y}|\mathcal{D}, \theta^{(t)}) \\
&= \sum_{y_1=1}^{m} \cdots \sum_{y_n=1}^{m} \sum_{i=1}^{n} \log p(x_i, y_i|\theta) \prod_{l=1}^{n} p(y_l|x_l, \theta^{(t)}) \\
&= \sum_{y_1=1}^{m} \cdots \sum_{y_n=1}^{m} \sum_{i=1}^{n} \log \left(w_{y_i} p(x_i|\theta_{y_i}) \right) \prod_{l=1}^{n} p(y_l|x_l, \theta^{(t)}).
\end{aligned}$$

After several simplification steps, that we omit for space reasons, the expectation of the likelihood can be written as

$$E[\log p(\mathcal{D}, \mathbf{y}|\theta)|\theta^{(t)}] = \sum_{i=1}^{n} \sum_{j=1}^{m} \log \left(w_j p(x_i|\theta_j) \right) p_{Y_i}(j|x_i, \theta^{(t)}),$$

from which we can see that $\mathbf{w}$ and $\{\theta_j\}_{j=1}^{m}$ can be separately found. In the final two steps, we will first derive the update rule for the mixing probabilities and then by assuming the mixing distributions are exponential, derive the update rules for their parameters.

To maximize $E[\log p(\mathcal{D}, \mathbf{y}|\theta)|\theta^{(t)}]$ with respect to $\mathbf{w}$, we observe that this is an instance of constrained optimization because it must hold that $\sum_{i=1}^{m} w_i = 1$. We will use the method of Lagrange multipliers; thus, for each $k \in \mathcal{Y}$ we need to solve

$$\frac{\partial}{\partial w_k}\left(\sum_{j=1}^{m}\log w_j\sum_{i=1}^{n}p_{Y_i}(j|x_i,\theta^{(t)})+\alpha\left(\sum_{j=1}^{m}w_j-1\right)\right)=0,$$

where α is the Lagrange multiplier. It is relatively straightforward to show that

$$w_k^{(t+1)}=\frac{1}{n}\sum_{i=1}^{n}p_{Y_i}(k|x_i,\theta^{(t)}). \tag{9.6}$$

Similarly, to find the solution for the parameters of the mixture distributions, we obtain that

$$\lambda_k^{(t+1)}=\frac{\sum_{i=1}^{n}p_{Y_i}(k|x_i,\theta^{(t)})}{\sum_{i=1}^{n}x_i p_{Y_i}(k|x_i,\theta^{(t)})} \tag{9.7}$$

for $k\in\mathcal{Y}$. As previously shown, we have

$$p_{Y_i}(k|x_i,\theta^{(t)})=\frac{w_k^{(t)}p(x_i|\lambda_k^{(t)})}{\sum_{j=1}^{m}w_j^{(t)}p(x_i|\lambda_j^{(t)})}, \tag{9.8}$$

which can be computed and stored as an $n\times m$ matrix. In summary, for the mixture of m exponential distributions, we summarize the EM algorithm by combining Eqs. (9.6-9.8) as follows:

1. Initialize $\lambda_k^{(0)}$ and $w_k^{(0)}$ for $\forall k\in\mathcal{Y}$
2. Set $t=0$
3. Repeat until convergence
   (a) $p_{Y_i}(k|x_i,\theta^{(t)})=\frac{w_k^{(t)}p(x_i|\lambda_k^{(t)})}{\sum_{j=1}^{m}w_j^{(t)}p(x_i|\lambda_j^{(t)})}$ for $\forall(i,k)$
   (b) $w_k^{(t+1)}=\frac{1}{n}\sum_{i=1}^{n}p_{Y_i}(k|x_i,\theta^{(t)})$
   (c) $\lambda_k^{(t+1)}=\frac{\sum_{i=1}^{n}p_{Y_i}(k|x_i,\theta^{(t)})}{\sum_{i=1}^{n}x_i p_{Y_i}(k|x_i,\theta^{(t)})}$
   (d) $t=t+1$
4. Report $\lambda_k^{(t)}$ and $w_k^{(t)}$ for $\forall k\in\mathcal{Y}$

Similar update rules can be obtained for different probability distributions; however, a separate derivatives have to be found.

Notice the difference between the CEM and the EM algorithms.

Identifiability

When estimating the parameters of a mixture, it is possible that for some parametric families one obtains multiple solutions. In other words,

$$p(x;\theta)=\sum_{j=1}^{m}w_j p(x;\theta_j),$$

but can also be expressed as

$$p(x;\theta') = \sum_{j=1}^{m'} w'_j p(x;\theta'_j),$$

The parameters are identifiable if

$$\sum_{j=1}^{m} w_j p(x;\theta_j) = \sum_{j=1}^{m'} w'_j p(x;\theta'_j),$$

implies that $m = m'$ for each $j \in \{1, 2, \ldots, m\}$ there exists some $l \in \{1, 2, \ldots, m\}$ such that $w_j = w'_l$ and $\theta_j = \theta'_l$.

Bibliography

[1] P Auer, M Herbster, and M K Warmuth. Exponentially many local minima for single neurons. In *Advances in Neural Information Processing Systems*, 1996.

[2] A Banerjee, S Merugu, I S Dhillon, and J Ghosh. Clustering with Bregman divergences. *Journal of Machine Learning Research*, 2005.

[3] Peter L Bartlett and Shahar Mendelson. Rademacher and Gaussian Complexities: Risk Bounds and Structural Results. In *Computational Learning Theory*. 2001.

[4] L on Bottou and Yann Le Cun. On-line learning for very large data sets. *Applied Stochastic Models in Business and Industry*, 2005.

[5] Léon Bottou. Online learning and stochastic approximations. *Online Learning and Neural Networks*, 1998.

[6] Olivier Bousquet, Stéphane Boucheron, and Gábor Lugosi. Introduction to Statistical Learning Theory. In *Advanced Lectures on Machine Learning*. 2004.

[7] Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani. *An Introduction to Statistical Learning*. Springer New York, 2013.

[8] Nathalie Japkowicz and Mohak Shah. Evaluating Learning Algorithms - A Classification Perspective. 2011.

[9] Sham M Kakade, Karthik Sridharan, and Ambuj Tewari. On the Complexity of Linear Prediction: Risk Bounds, Margin Bounds, and Regularization. In *Advances in Neural Information Processing Systems*, 2008.

[10] Lei Le and Martha White. Global optimization of factor models using alternating minimization. *arXiv.org*, 2016.

[11] Julien Mairal, Francis Bach, Jean Ponce, Guillermo Sapiro, and Andrew Zisserman. Supervised dictionary learning. In *Advances in Neural Information Processing Systems*, 2009.

[12] Bruno A Olshausen and David J Field. Sparse coding with an overcomplete basis set: a strategy employed by V1? *Vision Research*, 1997.

[13] Dinah Shender and John Lafferty. Computation-Risk Tradeoffs for Covariance-Thresholded Regression. *International Conference on Machine Learning*, 2013.

[14] Ajit P Singh and Geoffrey J Gordon. A unified view of matrix factorization models. In *European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases*, 2008.

[15] Larry Wasserman. *All of Statistics: A Concise Course in Statistical Inference*. Springer, 2004.

[16] M White. *Regularized factor models*. PhD thesis, University of Alberta, 2014.

Appendix A

Notation reference

A.1 Set notation

$\mathcal{X}$ A generic set of values. For example, $\mathcal{X} = \{0, 1\}$ is the set containing only 0 and 1, $\mathcal{X} = [0, 1]$ is the interval from 0 to 1 and $\mathcal{X} = \mathbb{R}$ is the real numbers.

$\mathcal{P}(\mathcal{X})$ The power set of $\mathcal{X}$, containing all possible subsets of $\mathcal{X}$.

$[a, b]$ Closed interval with $a < b$, including both a and b.

(a, b) Open interval with $a < b$, with neither a nor b in the set.

$(a, b]$ Open-closed interval with $a < b$, including b but not a.

$[a, b)$ Closed-open interval with $a < b$, including a but not b.

$a_1, \ldots, a_m$ A sequence of m items. Index variables over these sequences are usually the variables i, j or k. For example, $\sum_{i=1}^{m} a_i$ or, if each $\mathbf{a}_i$ is a vector of dimension d, then the double index $\sum_{i=1}^{m} \sum_{j=1}^{m} a_{ij}$.

A.2 Vector and matrix notation

x Unbold lower case variables are scalars.

$\mathbf{x}$ Bold lower case variables are vectors.

$\mathbf{X}$ Bold upper case variables are matrices. This looks like a multivariate random variable, $\boldsymbol{X}$, but the RV is italicized. Further, if the is hard to see, context will often make it clear when this is a multivariate random variable and when it is a matrix.

$\mathbf{X}^\top$ The transpose of the matrix. For two matrices $\mathbf{A}, \mathbf{B}$, $(\mathbf{AB})^\top = \mathbf{B}^\top \mathbf{A}^\top$.

$\mathbf{X}_{:j}$ The jth column of the matrix.

$\mathbf{X}_{i:}$ The ith row of the matrix.

A.3 Function notation

$f : D \to R$ The function is defined on domain D to range R, taking values $x \in D$ and sending them to $f(x) \in R$.

$\frac{df}{dx}(x)$ The derivative of a function at $x \in \mathcal{X}$, where $f : \mathcal{X} \to \mathbb{R}$ for $\mathcal{X} \subset \mathbb{R}$.

$\nabla f(\mathbf{x})$ The gradient of a function at $x \in \mathcal{X}$, where $f : \mathcal{X} \to \mathbb{R}$ for $\mathcal{X} \subset \mathbb{R}^d$.

A.4 Random variables and probabilities

X A univariate random variable is written in uppercase.

$\mathcal{X}$ The space of values for the random variable.

x Lower case variable is an instance or outcome, $x \in \mathcal{X}$

$\boldsymbol{X}$ A multivariate random variable is written bold uppercase.

$\mathbf{x}$ Lower case bold variable is a multivariate instance.

$\mathcal{N}(\mu, \sigma^2)$ A univariate Gaussian distribution, with parameters μ, σ^2.

$\sim$ indicates that a variable is distributed as e.g., $X \sim \mathcal{N}(\mu, \sigma^2)$.

A.5 Parameters and estimation

$\mathcal{D}$ A dataset, typically composed of n samples of multivariate inputs $\mathbf{X} \in \mathbb{R}^{n \times d}$ and univariate outputs $\mathbf{y} \in \mathbb{R}^n$ or multivariate outputs $\mathbf{Y} \in \mathbb{R}^{n \times m}$.

M Represents a generic model, to discuss general parameter estimation. For example, $M = \theta$ for some parameters θ, such as the mean of Gaussian distribution.

$\boldsymbol{\omega}$ The true parameters for the (generalized) linear regression and classification models, typically with $\boldsymbol{\omega} \in \mathbb{R}^d$.

$\mathbf{w}$ The approximated parameters for the (generalized) linear regression and classification models, typically with $\mathbf{w} \in \mathbb{R}^d$. When discussing $\mathbf{w}$ as the maximum likelihood solution on some data, we write $\mathbf{w}_{\text{ML}}(\mathcal{D})$, to indicate that the variability arises from $\mathcal{D}$.

$\max_{a \in \mathcal{B}} f(a)$ The maximum value of a function f across values a in a set $\mathcal{B}$.

$\text{argmax}_{a \in \mathcal{B}} f(a)$ The item a in set $\mathcal{B}$ that produces the maximum value $f(a)$.

A.6 Norms

$\|\mathbf{x}\|$ A norm on $\mathbf{x}$.

$\|\mathbf{x}\|_2$ The ℓ_2 norm on a vector, $\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^{d} x_i^2}$.

$\|\mathbf{x}\|_2^2$ The squared ℓ_2 norm on a vector, $\|\mathbf{x}\|_2^2 = \sum_{i=1}^{d} x_i^2$.

$\|\mathbf{x}\|_p$ The general ℓ_p norm on a vector, $\|\mathbf{x}\|_p = (\sum_{i=1}^{d} x_i^p)^{1/p}$.

$\|\mathbf{X}\|_F$ The Frobenius norm of a matrix, $\|\mathbf{X}\|_F = \sqrt{\sum_{i=1}^{n}\sum_{j=1}^{d} X_{ij}^2} = \sqrt{\sum_{i=1}^{n} \|X_{i:}\|_2^2} = \sqrt{\sum_{j=1}^{d} \|X_{:j}\|_2^2}$.

A.7 Useful formulas and rules

$$\log\left(\frac{x}{y}\right) = \log(x) - \log(y)$$

$$\log\left(x^y\right) = y\log(x)$$

$$\sum_{i=1}^{m} a_i \int_{\mathcal{X}} f_i(x)p(x)dx = \int_{\mathcal{X}} \sum_{i=1}^{m} a_i f_i(x)p(x)dx \qquad \triangleright \text{Can bring sum into integral}$$

$$\frac{d}{dx}\int_{\mathcal{X}} f(x)p(x)dx = \int_{\mathcal{X}} \frac{d}{dx} f(x)p(x)dx \qquad \triangleright \text{Can (almost always) bring derivative into integral}$$

Appendix B

Optimization background

B.1 First-order gradient descent

First-order gradient descent involves using only information about the first gradient to find the minimum of a function. To obtain gradients, it is useful to have gradient rules for vectors and matrices. You are familiar with rules for derivatives with univariate variables, such as $\frac{d}{dx}x^2 = 2x$. Such rules similarly exist for partial derivatives for multivariate variables, where

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial \mathbf{x}_1}(\mathbf{x}) & \frac{\partial f}{\partial \mathbf{x}_2}(\mathbf{x}) & \dots & \frac{\partial f}{\partial \mathbf{x}_d}(\mathbf{x}) \end{bmatrix}.$$

Some of these rules are summarized in Table B.1. This list is not comprehensive, but does enable some additional rules to be derived. For example, to obtain the derivative for the function $f(\mathbf{x}) = \mathbf{x}^\top \mathbf{A}$, one can first obtain the derivative for $f(\mathbf{x})^\top = \mathbf{A}^\top \mathbf{x}$ and then take its transpose because

$$\big(\nabla f(\mathbf{x})\big)^\top = \nabla\big(f(\mathbf{x})^\top\big).$$

Therefore, because $\nabla f(\mathbf{x})^\top = \mathbf{A}^\top$, we get that $\nabla f(\mathbf{x}) = \mathbf{A}$.

$f(\mathbf{x})$	$\frac{\partial f}{\partial \mathbf{x}}$
$\mathbf{x}^\top \mathbf{x}$	$2\mathbf{x}$
$\mathbf{A}\mathbf{x}$	$\mathbf{A}$
$\mathbf{x}^\top \mathbf{A}\mathbf{x}$	$\mathbf{A}\mathbf{x} + \mathbf{A}^\top \mathbf{x}$

Table B.1: Useful derivative formulas of vectors with respect to vectors. The derivative of vector-valued function $f : \mathbb{R}^{d\times 1} \to \mathbb{R}^{m\times 1}$ with respect to vector $\mathbf{x} \in \mathbb{R}^{d\times 1}$ is an $m \times d$ matrix $\mathbf{M}$ with components $M_{ij} = \partial y_j / \partial x_i$, $i \in \{1, 2, \dots, d\}$ and $j \in \{1, 2, \dots, m\}$. A derivative of scalar with respect to a vector, where $m = 1$, is a special case of this situation that results in an $d \times 1$ column vector. Note that in the table, m is not the same for each row. For example, $f(\mathbf{x}) = \mathbf{x}^\top \mathbf{x}$ is a scalar, whereas for a general matrix $\mathbf{A} \in \mathbb{R}^{m\times d}$, $f(\mathbf{x}) = \mathbf{A}\mathbf{x}$ is a m-dimensional vector.

B.2 Second-order optimization

A function $f(x)$ in the neighborhood of point x_0, can be approximated using the Taylor series as

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n,$$

where $f^{(n)}(x_0)$ is the n-th derivative of function $f(x)$ evaluated at point x_0. Also, $f(x)$ is considered to be infinitely differentiable. For practical reasons, we will approximate this function using the first three terms of the series as

$$f(x) \approx f(x_0) + (x - x_0)f'(x_0) + \frac{1}{2}(x - x_0)^2 f''(x_0).$$

The optimum of this function can be found by finding the first derivative and setting it to zero (technically, one should check the second derivative as well)

$$f'(x) \approx f'(x_0) + (x - x_0)f''(x_0) = 0.$$

Solving this equation for x gives us

$$x = x_0 - \frac{f'(x_0)}{f''(x_0)}.$$

Note that the approach assumes that a good enough solution x_0 already exists. However, this equation, also provides a basis for an iterative process in finding the optimum of function $f(x)$. For example, if $x^{(i)}$ is the value of x in the i-th step, then the value in step $i+1$ can be obtained as

$$x^{(i+1)} = x^{(i)} - \frac{f'(x^{(i)})}{f''(x^{(i)})}. \tag{B.1}$$

This method is called the Newton-Raphson method of optimization. We can generalize this approach to functions of vector variables $\mathbf{x} = (x_1, x_2, \ldots, x_k)$. The Taylor approximation for a vector function can be written as

$$f(\mathbf{x}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^T \cdot (\mathbf{x} - \mathbf{x}_0) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^T \cdot H_{f(\mathbf{x}_0)} \cdot (\mathbf{x} - \mathbf{x}_0),$$

where

$$\nabla f(\mathbf{x}) = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, ..., \frac{\partial f}{\partial x_k} \right)$$

is the gradient of function f and

$$H_{f(\mathbf{x})} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_k} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & & \\ \vdots & & \ddots & \\ \frac{\partial^2 f}{\partial x_k \partial x_1} & & & \frac{\partial^2 f}{\partial x_k^2} \end{bmatrix}$$

is the Hessian matrix of function f. Here, the gradient of f and its Hessian are evaluated at point $\mathbf{x}_0$. Consequently, Eq. B.1 is modified into the following form

$$\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \left(H_{f(\mathbf{x}^{(i)})}\right)^{-1} \cdot \nabla f(\mathbf{x}^{(i)}), \tag{B.2}$$

In Eq. B.2, both gradient and Hessian are evaluated at point $\mathbf{x}^{(i)}$.

Appendix C

Linear algebra background

C.1 An Algebraic Perspective

Another powerful tool for analyzing and understanding linear regression comes from linear and applied linear algebra. In this section we take a detour to address fundamentals of linear algebra and then apply these concepts to deepen our understanding of regression. In linear algebra, we are frequently interested in solving the following set of equations, given below in a matrix form

$$\mathbf{A}\mathbf{x} = \mathbf{b}. \tag{C.1}$$

Here, $\mathbf{A}$ is an $m \times n$ matrix, $\mathbf{b}$ is an $m \times 1$ vector, and $\mathbf{x}$ is an $n \times 1$ vector that is to be found. All elements of $\mathbf{A}$, $\mathbf{x}$, and $\mathbf{b}$ are considered to be real numbers. We shall start with a simple scenario and assume $\mathbf{A}$ is a square, 2×2 matrix. This set of equations can be expressed as

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 &= b_1 \\ a_{21}x_1 + a_{22}x_2 &= b_2 \end{aligned}$$

For example, we may be interested in solving

$$\begin{aligned} x_1 + 2x_2 &= 3 \\ x_1 + 3x_2 &= 5 \end{aligned}$$

This is a convenient formulation when we want to solve the system, e.g. by Gaussian elimination. However, it is not a suitable formulation to understand the question of the existence of solutions. In order for us to do this, we briefly review the basic concepts in linear algebra.

C.1.1 The four fundamental subspaces

The objective of this section it to briefly review the *four fundamental subspaces* in linear algebra (column space, row space, nullspace, left nullspace) and their mutual relationship. We shall start with our example from above and write the system of linear equations as

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix} x_1 + \begin{bmatrix} 2 \\ 3 \end{bmatrix} x_2 = \begin{bmatrix} 3 \\ 5 \end{bmatrix}.$$

We can see now that by solving $\mathbf{A}\mathbf{x} = \mathbf{b}$ we are looking for the right amounts of vectors $(1, 1)$ and $(2, 3)$ so that their linear combination produces $(3, 5)$; these amounts are $x_1 = -1$ and $x_2 = 2$. Let us define $\mathbf{a}_1 = (1, 1)$ and $\mathbf{a}_2 = (2, 3)$ to be the column vectors of $\mathbf{A}$; i.e. $\mathbf{A} = [\mathbf{a}_1\ \mathbf{a}_2]$. Thus, $\mathbf{A}\mathbf{x} = \mathbf{b}$ will be solvable whenever $\mathbf{b}$ can be expressed as a linear combination of the column vectors $\mathbf{a}_1$ and $\mathbf{a}_2$.

All linear combinations of the columns of matrix $\mathbf{A}$ constitute the *column space* of $\mathbf{A}$, $C(\mathbf{A})$, with vectors $\mathbf{a}_1 \ldots \mathbf{a}_n$ being a basis of this space. Both $\mathbf{b}$ and $C(\mathbf{A})$ lie in the m-dimensional space $\mathbb{R}^m$. Therefore, what $\mathbf{A}\mathbf{x} = \mathbf{b}$ is saying is that $\mathbf{b}$ must lie in the column space of $\mathbf{A}$ for the equation to have

solutions. In the example above, if columns of $\mathbf{A}$ are linearly independent[1], the solution is unique, i.e. there exists only one linear combination of the column vectors that will give $\mathbf{b}$. Otherwise, because $\mathbf{A}$ is a square matrix, the system has no solutions. An example of such a situation is

$$\begin{bmatrix} 1 & 2 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 5 \end{bmatrix},$$

where $\mathbf{a}_1 = (1, 1)$ and $\mathbf{a}_2 = (2, 2)$. Here, $\mathbf{a}_1$ and $\mathbf{a}_2$ are (linearly) dependent because $2\mathbf{a}_1 - \mathbf{a}_2 = 0$. There is a deep connection between the spaces generated by a set of vectors and the properties of the matrix A. For now, using the example above, it suffices to say that if $\mathbf{a}_1$ and $\mathbf{a}_2$ are independent the matrix $\mathbf{A}$ is non-singular (singularity can be discussed only for square matrices), that is of full rank.

In an equivalent manner to the column space, all linear combinations of the rows of $\mathbf{A}$ constitute the *row space*, denoted by $C(\mathbf{A}^\top)$, where both $\mathbf{x}$ and $C(\mathbf{A}^\top)$ are in $\mathbb{R}^n$. All solutions to $\mathbf{Ax} = \mathbf{0}$ constitute the *nullspace* of the matrix, $N(\mathbf{A})$, while all solutions of $\mathbf{A}^\top\mathbf{y} = \mathbf{0}$ constitute the so-called *left nullspace* of $\mathbf{A}$, $N(\mathbf{A}^\top)$. Clearly, $C(\mathbf{A})$ and $N(\mathbf{A}^\top)$ are embedded in $\mathbb{R}^m$, whereas $C(\mathbf{A}^\top)$ and $N(\mathbf{A})$ are in $\mathbb{R}^n$. However, the pairs of subspaces are orthogonal (vectors $\mathbf{u}$ and $\mathbf{v}$ are orthogonal if $\mathbf{u}^\top\mathbf{v} = 0$); that is, any vector in $C(\mathbf{A})$ is orthogonal to all vectors from $N(\mathbf{A}^\top)$ and any vector in $C(\mathbf{A}^\top)$ is orthogonal to all vectors from $N(\mathbf{A})$. This is easy to see: if $\mathbf{x} \in N(\mathbf{A})$, then by definition $\mathbf{Ax} = \mathbf{0}$, and thus each row of $\mathbf{A}$ is orthogonal to $\mathbf{x}$. If each row is orthogonal to $\mathbf{x}$, then so are all linear combinations of rows.

Orthogonality is a key property of the four subspaces, as it provides useful decomposition of vectors $\mathbf{x}$ and $\mathbf{b}$ from Eq. (C.1) with respect to $\mathbf{A}$ (we will exploit this in the next Section). For example, any $\mathbf{x} \in \mathbb{R}^n$ can be decomposed as

$$\mathbf{x} = \mathbf{x}_r + \mathbf{x}_n,$$

where $\mathbf{x}_r \in C(\mathbf{A}^\top)$ and $\mathbf{x}_n \in N(\mathbf{A})$, such that $\|\mathbf{x}\|_2^2 = \|\mathbf{x}_r\|_2^2 + \|\mathbf{x}_n\|_2^2$. Similarly, every $\mathbf{b} \in \mathbb{R}^m$ can be decomposed as

$$\mathbf{b} = \mathbf{b}_c + \mathbf{b}_l,$$

where $\mathbf{b}_c \in C(\mathbf{A})$, $\mathbf{b}_l \in N(\mathbf{A}^\top)$, and $\|\mathbf{b}\|_2^2 = \|\mathbf{b}_c\|_2^2 + \|\mathbf{b}_l\|_2^2$.

We mentioned above that the properties of fundamental spaces are tightly connected with the properties of matrix $\mathbf{A}$. To conclude this section, let us briefly discuss the *rank* of a matrix and its relationship with the dimensions of the fundamental subspaces. The *basis* of the space is the smallest set of vectors that span the space (this set of vectors is not unique). The size of the basis is also called the dimension of the space. In the example at the beginning of this subsection, we had a two dimensional column space with basis vectors $\mathbf{a}_1 = (1, 1)$ and $\mathbf{a}_2 = (2, 3)$. On the other hand, for $\mathbf{a}_1 = (1, 1)$ and $\mathbf{a}_2 = (2, 2)$ we had a one dimensional column space, i.e. a line, fully determined by any of the basis vectors. Unsurprisingly, the dimension of the space spanned by column vectors equals the *rank* of matrix $\mathbf{A}$. One of the fundamental results in linear algebra is that the rank of $\mathbf{A}$ is identical to the dimension of $C(\mathbf{A})$, which in turn is identical to the dimension of $C(\mathbf{A}^\top)$.

C.1.2 Minimizing $\|\mathbf{Ax} - \mathbf{b}\|_2$

Let us now look again at the solutions to $\mathbf{Ax} = \mathbf{b}$. In general, there are three different outcomes:

1. there are no solutions to the system
2. there is a unique solution to the system, and
3. there are infinitely many solutions.

[1]As a reminder, two vectors are independent if their linear combination is only zero when both x_1 and x_2 are zero.

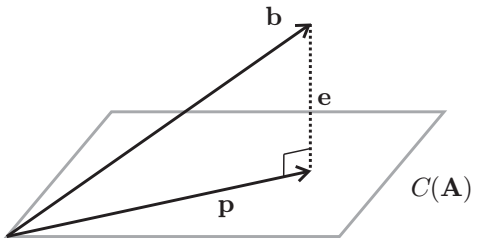


Figure C.1: Illustration of the projection of vector $\mathbf{b}$ *to the column space of matrix* $\mathbf{A}$*. Vectors* $\mathbf{p}$ *(*$\mathbf{b}_c$*) and* $\mathbf{e}$ *(*$\mathbf{b}_l$*) represent the projection point and the error, respectively.*

These outcomes depend on the relationship between the rank (r) of $\mathbf{A}$ and dimensions m and n. We already know that when $r = m = n$ (square, invertible, full rank matrix $\mathbf{A}$) there is a unique solution to the system, but let us investigate other situations. Generally, when $r = n < m$ (full column rank), the system has either one solution or no solutions, as we will see momentarily. When $r = m < n$ (full row rank), the system has infinitely many solutions. Finally, in cases when $r < m$ and $r < n$, there are either no solutions or there are infinitely many solutions. Because $\mathbf{Ax} = \mathbf{b}$ may not be solvable, we generalize solving $\mathbf{Ax} = \mathbf{b}$ to minimizing $\|\mathbf{Ax} - \mathbf{b}\|_2$. In such a way, all situations can be considered in a unified framework.

Let us consider the following example

$$\mathbf{A} = \begin{bmatrix} 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix}, \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix},$$

which illustrates an instance where we are unlikely to have a solution to $\mathbf{Ax} = \mathbf{b}$, unless there is some constraint on b_1, b_2, and b_3; here, the constraint is $b_3 = 2b_2 - b_1$. In this situation, $C(\mathbf{A})$ is a 2D plane in $\mathbb{R}^3$ spanned by the column vectors $\mathbf{a}_1 = (1, 1, 1)$ and $\mathbf{a}_2 = (2, 3, 4)$. If the constraint on the elements of $\mathbf{b}$ is not satisfied, our goal is to try to find a point in $C(\mathbf{A})$ that is closest to $\mathbf{b}$**.** This happens to be the point where $\mathbf{b}$ is projected to $C(\mathbf{A})$, as shown in Figure C.1. We will refer to the projection of $\mathbf{b}$ to $C(\mathbf{A})$ as $\mathbf{p}$. Now, using the standard algebraic notation, we have the following equations

$$\mathbf{b} = \mathbf{p} + \mathbf{e}$$
$$\mathbf{p} = \mathbf{Ax}$$

Since $\mathbf{p}$ and $\mathbf{e}$ are orthogonal, we know that $\mathbf{p}^\top \mathbf{e} = 0$. Let us now solve for $\mathbf{x}$

$$(\mathbf{Ax})^\top (\mathbf{b} - \mathbf{Ax}) = 0$$
$$\mathbf{x}^\top \mathbf{A}^\top \mathbf{b} - \mathbf{x}^\top \mathbf{A}^\top \mathbf{Ax} = 0$$
$$\mathbf{x}^\top \left(\mathbf{A}^\top \mathbf{b} - \mathbf{A}^\top \mathbf{Ax}\right) = 0$$

and thus

$$\mathbf{x}^* = \left(\mathbf{A}^\top \mathbf{A}\right)^{-1} \mathbf{A}^\top \mathbf{b}.$$

This is exactly the same solution as one that minimized the sum of squared errors and maximized the likelihood. The matrix

$$\mathbf{A}^\dagger = \left(\mathbf{A}^\top \mathbf{A}\right)^{-1} \mathbf{A}^\top$$

is called the Moore-Penrose pseudo-inverse or simply a pseudo-inverse. This is an important matrix because it always exists and is unique, even in situations when the inverse of $\mathbf{A}^\top \mathbf{A}$ does not exist.

This happens when $\mathbf{A}$ has dependent columns (technically, $\mathbf{A}$ and $\mathbf{A}^\top\mathbf{A}$ will have the same nullspace that contains more than just the origin of the coordinate system; thus the rank of $\mathbf{A}^\top\mathbf{A}$ is less than n). Let us for a moment look at the projection vector $\mathbf{p}$. We have

$$\begin{aligned}\mathbf{p} &= \mathbf{A}\mathbf{x} \\ &= \mathbf{A}\left(\mathbf{A}^\top\mathbf{A}\right)^{-1}\mathbf{A}^\top\mathbf{b},\end{aligned}$$

where $\mathbf{A}\left(\mathbf{A}^\top\mathbf{A}\right)^{-1}\mathbf{A}^\top$ is the matrix that projects $\mathbf{b}$ to the column space of $\mathbf{A}$.

While we arrived at the same result as in previous sections, the tools of linear algebra allow us to discuss OLS regression at a deeper level. Let us examine for a moment the existence and multiplicity of solutions to

$$\arg\min_{\mathbf{x}} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2 . \tag{C.2}$$

Clearly, the solution to this problem always exists. However, we shall now see that the solution to this problem is generally not unique and that it depends on the rank of $\mathbf{A}$. Consider $\mathbf{x}$ to be one solution to Eq. (C.2). Recall that $\mathbf{x} = \mathbf{x}_r + \mathbf{x}_n$ and that it is multiplied by $\mathbf{A}$; thus any vector $\mathbf{x} = \mathbf{x}_r + \alpha\mathbf{x}_n$, where $\alpha \in \mathbb{R}$, is also a solution. Observe that $\mathbf{x}_r$ is common to all such solutions; if you cannot see it, assume there exists another vector from the row space and show that it is not possible. If the columns of $\mathbf{A}$ are independent, the solution is unique because the nullspace contains only the origin. Otherwise, there are infinitely many solutions. In such cases, what exactly is the solution found by projecting $\mathbf{b}$ to $C(\mathbf{A})$? Let us look at it:

$$\begin{aligned}\mathbf{x}^* &= \mathbf{A}^\dagger\mathbf{b} \\ &= \left(\mathbf{A}^\top\mathbf{A}\right)^{-1}\mathbf{A}^\top(\mathbf{p}+\mathbf{e}) \\ &= \left(\mathbf{A}^\top\mathbf{A}\right)^{-1}\mathbf{A}^\top\mathbf{p} \\ &= \mathbf{x}_r,\end{aligned}$$

as $\mathbf{p} = \mathbf{A}\mathbf{x}_r$. Given that $\mathbf{x}_r$ is unique, the solution found by the least squares optimization is the one that simultaneously minimizes $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2$ and $\|\mathbf{x}\|_2$ (observe that $\|\mathbf{x}\|_2$ is minimized because the solution ignores any component from the nullspace). Thus, the OLS regression problem is sometimes referred to as the minimum-norm least-squares problem.

Let us now consider situations where $\mathbf{A}\mathbf{x} = \mathbf{b}$ has infinitely many solutions, i.e. when $\mathbf{b} \in C(\mathbf{A})$. This usually arises when $r \leq m < n$. Here, because $\mathbf{b}$ is already in the column space of $\mathbf{A}$, the only question is what particular solution $\mathbf{x}$ will be found by the minimization procedure. As we have seen above, the outcome of the minimization process is the solution with the minimum L_2 norm $\|\mathbf{x}\|_2$.

To summarize, the goal of the OLS regression problem is to solve $\mathbf{x}\mathbf{w} = \mathbf{y}$, if it is solvable. When $k < n$ this is not a realistic scenario in practice. Thus, we relaxed the requirement and tried to find the point in the column space $C(\mathbf{x})$ that is closest to $\mathbf{y}$. This turned out to be equivalent to minimizing the sum of square errors (or Euclidean distance) between n-dimensional vectors $\mathbf{X}\mathbf{w}$ and $\mathbf{y}$. It also turned out to be equivalent to the maximum likelihood solution presented in Section 4.1. When $n < k$, a usual situation in practice is that there are infinitely many solutions. In these situations, our optimization algorithm will find the one with the minimum L_2 norm.

Appendix D

Details on unsupervised representation approaches using factorization

There are many variants of unsupervised learning algorithms that actually correspond to factorizing the data matrix, which we summarize in in Table D.1. In many cases, they simply correspond to defining an interesting kernel on $\mathbf{X}$, and then factorizing that kernel (i.e., kernel PCA). If the entry is empty, this specifies no regularization and no constraints. For a more complete list, see [14] and [16]). As with the regression setting, we can generalize this Euclidean loss to any convex loss

$$L_x(\mathbf{H}, \mathbf{D}, \mathbf{X}) = \sum_{i=1}^{n} L_x(\mathbf{H}_{i:}\mathbf{D}, \mathbf{X}_{i:})$$

where above we used

$$L_x(\mathbf{H}, \mathbf{D}, \mathbf{X}) = \sum_{i=1}^{n} \|\mathbf{H}_{i:}\mathbf{D} - \mathbf{X}_{i:}\|_2^2 = \|\mathbf{HD} - \mathbf{X}\|_F^2 .$$

Algorithms to learn dictionaries

Our focus remains on prediction, and so we would like to use these representations for supervised (or semi-supervised) learning. We use a two-stage approach, where first the new representation is learned in an unsupervised way and then used with supervised learning algorithms. These two stages could be combined into one step with supervised dictionary learning; see [11] for a discussion about this more advanced approach.

The most common strategy to learn these dictionary models is to do an alternating minimization over the variables. The optimization over $\mathbf{D}$ and $\mathbf{H}$ is not jointly convex; however, it is convex in each variable separately. The strategy is to fix one variable, say $\mathbf{H}$, and descend in the other, say $\mathbf{D}$, and then switch, fixing $\mathbf{D}$ and descending in $\mathbf{H}$. This alternating minimization continues until the convergence. Though this is a nonconvex optimization, there is recent evidence that this procedure actually returns the global minimum (see e.g. [10]). We summarize this procedure in Algorithm 4.

Once the dictionary $\mathbf{D}$ and new representation $\mathbf{H}$ have been learned, we can learn the supervised weights $\mathbf{W} \in \mathbb{R}^{k \times m}$ to obtain $\mathbf{HW} \approx \mathbf{Y}$. This can be done with any of the linear regression or classification approaches we have learned so far.

Finally, we need to know how to use these learned models for out-of-sample prediction (i.e., for new samples). The matrices $\mathbf{D}$ and $\mathbf{W}$ contain all the necessary information to perform out-of-sample prediction, and $\mathbf{H}$ does not need to be stored, because it was the representation specific to the training data. For a new sample $\mathbf{x}_{\text{new}}$, the representation can be obtained using

$$\mathbf{h}_{\text{new}} = \operatorname*{argmin}_{\mathbf{h} \in \mathbb{R}^k} L_x(\mathbf{hD}, \mathbf{x}).$$

With the representation for this sample, we can then predict $f(\mathbf{h}_{\text{new}}\mathbf{W})$.

Algorithm	**Loss and constraints**
CCA $\equiv$ orthonormal PLS	$\left\| \begin{bmatrix} \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1} \\ \mathbf{Y}(\mathbf{Y}^\top\mathbf{Y})^{-1} \end{bmatrix} - \mathbf{HD} \right\|_F^2$
Isomap	$\|\mathbf{K} - \mathbf{HD}\|_F^2$ $\mathbf{K} = -\frac{1}{2}(\mathbf{I} - \mathbf{ee}')\mathbf{S}(\mathbf{I} - \mathbf{ee}')$ with $\mathbf{S}_{i,j} = \|\mathbf{X}_{i:} - \mathbf{X}_{j:}\|$
K-means clustering	$\|\mathbf{X} - \mathbf{HD}\|_F^2$ with $\mathbf{H} \in \{0,1\}^{n \times k}$, $\mathbf{H1} = \mathbf{1}$
K-medians clustering	$\|\mathbf{X} - \mathbf{HD}\|_{1,1}$ with $\mathbf{H} \in \{0,1\}^{n \times k}$, $\mathbf{H1} = \mathbf{1}$
Laplacian eigenmaps $\equiv$ Kernel LPP	$\|\mathbf{K} - \mathbf{HD}\|_F^2$ for $\mathbf{K} = \mathbf{L}^\dagger$
Metric multi-dimensional scaling	$\|\mathbf{K} - \mathbf{HD}\|_F^2$ for isotropic kernel $\mathbf{K}$
Normalized-cut	$\left\|(\mathbf{\Lambda}^{-1}\mathbf{X} - \mathbf{HD})\mathbf{\Lambda}^{1/2}\right\|_F^2$ with $\mathbf{H} \in \{0,1\}^{n \times k}$, $\mathbf{H1} = \mathbf{1}$
Partial least squares	$\|\mathbf{XY}' - \mathbf{DH}\|_F^2$
PCA	$\|\mathbf{X} - \mathbf{HD}\|_F^2$
Kernel PCA	$\|\mathbf{K} - \mathbf{HD}\|_F^2$
Ratio cut	$\|\mathbf{K} - \mathbf{HD}\|_F^2$ for $\mathbf{K} = \mathbf{L}^\dagger$

Figure D.1: Unsupervised learning algorithms that correspond to a matrix factorization.

Algorithm 4: Alternating minimization for dictionary learning

Input:

inner dimension k
loss L, where $\mathrm{L}(\mathbf{HD}) = L_x(\mathbf{H}, \mathbf{D}, \mathbf{X})$
R_D, the regularizer on $\mathbf{D}$
R_H, the regularizer on $\mathbf{H}$
the regularization weight λ
convergence tolerance
fixed positive step-sizes η_D, η_H
dataset $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$

Initialization:

$\mathbf{D}, \mathbf{H} \leftarrow$ full-rank random matrices with inner dimension k
prevobj $\leftarrow \infty$

Loop until convergence within tolerance or reach maximum number of iterations:

Update $\mathbf{D}$ using one step of gradient descent
Update $\mathbf{H}$ using one step of gradient descent
currentobj $\leftarrow \mathrm{L}(\mathbf{HD}) + \lambda R_D(\mathbf{D}) + \frac{\lambda}{n} R_H(\mathbf{H})$
If $|\text{currentobj} - \text{prevobj}| <$ tolerance, Then break
prevobj $\leftarrow$ currentobj

Output:

$\mathbf{D}, \mathbf{H}$