Basics of Machine Learning

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Notation Reference

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 set of real numbers. Depending on occasion, symbols such as A, B, Ω, and others will also be used as sets.

$\mathcal{P}(\mathcal{X})$ The power set of $\mathcal{X}$, a set 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.

Vector and matrix notation

x Unbold lowercase variables are generally scalars. However, when $x \in \mathcal{X}$, where $\mathcal{X}$ is not specified, x may imdicate a vector, a structured object such as graph, etc.

$\mathbf{x}$ Bold lowercase variables are vectors. By default, vectors are column vectors.

$\mathbf{X}$ Bold uppercase variables are matrices. This looks like a multivariate random variable, $\boldsymbol{X}$, but the random variable is italicized. It will often be clear from context when this is a multivariate random variable and when it is a matrix.

$\mathbf{X}^\top$ The transpose of the matrix. For two matrices $\mathbf{A}$ and $\mathbf{B}$, it holds that

$$(\mathbf{AB})^\top = \mathbf{B}^\top \mathbf{A}^\top.$$

An $n \times d$ matrix consisting of n vectors each of dimension d can be expressed as

$$\mathbf{X} = [\mathbf{x}_1 \, \mathbf{x}_2 \, \ldots \, \mathbf{x}_n]^\top.$$

$\mathbf{X}_{i:}$ The i-th row of the matrix. A row vector.

$\mathbf{X}_{:j}$ The j-th column of the matrix. A column vector.

Tuples, vectors, and sequences

$(x_1, x_2, \ldots, x_d)$ A tuple; i.e., an ordered list of d elements. When $(x_1, x_2, \ldots, x_d) \in \mathbb{R}^d$, the tuple will be treated as a column vector $\mathbf{x} = [x_1\, x_2\, \ldots\, x_d]^\top$.

$a_1, \ldots, a_m$ 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 $\sum_{i=1}^m \sum_{j=1}^d a_{ij}$.

Function notation

$f : \mathcal{X} \to \mathcal{Y}$ The function is defined on domain $\mathcal{X}$ to co-domain $\mathcal{Y}$, taking values $x \in \mathcal{X}$ and sending them to $f(x) \in \mathcal{Y}$.

$\frac{df}{dx}(x)$ 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 $\mathbf{x} \in \mathcal{X}$, where $f : \mathcal{X} \to \mathbb{R}$ for $\mathcal{X} \subset \mathbb{R}^d$. It holds that

$$\nabla f(\mathbf{x}) = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, ..., \frac{\partial f}{\partial x_d}\right).$$

$\ell : \mathbb{R}^d \to \mathbb{R}$ A loss function indicating the error in prediction incurred by the given weights, $\ell(\mathbf{w})$. If subscripted, ℓ_i typically indicates the loss on the ith instance, with $\ell(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^n \ell_i(\mathbf{w})$ for n instances.

$c : \mathbb{R}^d \to \mathbb{R}$ A generic objective function, that we want to minimize, for the learned variable $\mathbf{w}$. This could be, for example, a loss plus a regularizer.

Random variables and probabilities

X A univariate random variable is written in uppercase.

$\mathcal{X}$ The space of values for the random variable.

x Lowercase variable is an instance or outcome, $x \in \mathcal{X}$.

$\boldsymbol{X}$ A multivariate random variable is written bold uppercase.

$\boldsymbol{x}$ Lowercase bold variable is a multivariate instance. In particular cases, when the variable value is treated as a vector, we will use $\mathbf{x}$.

$\mathcal{N}(\mu, \sigma^2)$ A univariate Gaussian distribution, with parameters μ, σ^2.

$\sim$ indicates that a variable is distributed as e.g., $X \sim \mathcal{N}(\mu, \sigma^2)$.

Parameters and estimation

$\mathcal{D}$ A data set, typically composed of n elements of multivariate inputs $\mathbf{X} \in \mathbb{R}^{n\times d}$ and univariate outputs $\mathbf{y} \in \mathbb{R}^n$ or multivariate outputs $\mathbf{Y} \in \mathbb{R}^{n\times m}$. The data set will also be referred to as a set of indexed tuples; i.e., $\mathcal{D} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), ..., (\boldsymbol{x}_n, y_n)\}$.

$\mathcal{F}$ The *function class* or *hypothesis space*. Our learning algorithms will be restricted implicitly to selecting a function from this set. For example, in linear regression, our function class is $\mathcal{F} = \{f : \mathbb{R}^d \to \mathbb{R} \mid f(\mathbf{x}) = \mathbf{x}^\top \mathbf{w} for some \mathbf{w} \in \mathbb{R}^d\}$.

$\boldsymbol{\omega}$ 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 $\mathbf{w}_{\mathrm{ML}}(\mathcal{D})$, to indicate that the variability arises from $\mathcal{D}$.

$\max_{a\in\mathcal{B}} c(a)$ The maximum value of a function c across values a in a set $\mathcal{B}$.

$\mathrm{argmax}_{a\in\mathcal{B}} c(a)$ The item a in set $\mathcal{B}$ that produces the maximum value $c(a)$.

Norms

$\|\mathbf{x}\|$ A norm on $\mathbf{x}$.

$\|\mathbf{x}\|_2$ The ℓ_2 norm on a vector, $\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^d x_i^2}$. This norm gives the Euclidean distance from the origin of the coordinate system to $\mathbf{x}$; that is, it is the length of vector $\mathbf{x}$.

$\|\mathbf{x}\|_2^2$ 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, $\|\mathbf{x}\|_p = (\sum_{i=1}^d |x|_i^p)^{1/p}$.

Useful formulas and rules

$$\log\left(\frac{x}{y}\right) = \log(x) - \log(y)$$

$$\log\left(x^y\right) = y\log(x)$$

$$\sum_{i=1}^{m} a_i \int_{\mathcal{X}} f_i(x)p(x)dx = \int_{\mathcal{X}} \sum_{i=1}^{m} a_i f_i(x)p(x)dx \qquad \triangleright \text{ Can bring sum into integral}$$

$$\frac{d}{dx}\int_{\mathcal{X}} f(x)p(x)dx = \int_{\mathcal{X}} \frac{d}{dx} f(x)p(x)dx \qquad \triangleright \text{ Can (almost always) bring derivative into integral}$$

Chapter 1

A First Step in Machine Learning: Motivating a Probabilistic Formulation

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 techniques learn 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, for example by trying to find a function f that results in a small difference between the prediction, $f(\mathbf{x}_i)$, and the actual price, y_i, for each house.

We can formalize this as an optimization problem. Imagine we have some space of possible functions, $\mathcal{F}$, from which we can select our function f. For a simple 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

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

As we will see later, this optimization problem is simple to solve for linear functions. 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 1.1.

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 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

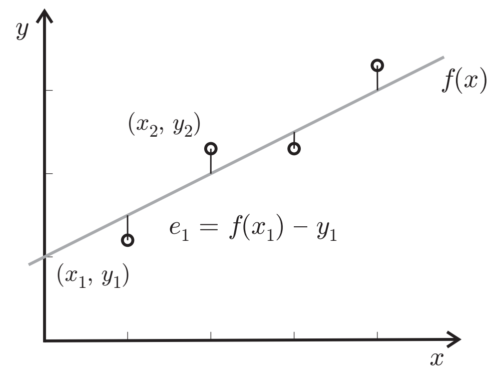


Figure 1.1: An example of a linear regression fitting on data set $\mathcal{D} = \{(1, 1.2), (2, 2.3), (3, 2.3), (4, 3.3)\}$. *The task of the optimization process is to find the best linear function* $f(x) = w_0 + w_1 x$ *so that the sum of squared errors* $e_1^2 + e_2^2 + e_3^2 + e_4^2$ *is minimized.*

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 2

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), "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—rather we have *partial observability*. 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.

The techniques of probabilistic modeling provide a formalism for dealing with such repetitive experiments influenced by a number of external factors over which we have little control or knowledge. With such a formalism, we can better understand and improve how we make predictions, because we can more clearly specify our assumptions about our uncertainty and explicitly reason about possible outcomes. In this chapter, we introduce probabilities and probability theory, from the beginning. Because probability is such a fundamental concept in machine learning, it is worth understanding where it comes from. Nonetheless, following the spirit of these notes, the treatment will be brief and focus mostly on what is needed to understand the development in following chapters.

2.1 Probability Theory and Random Variables

Probability theory is as a branch of mathematics that deals with measuring the likelihood of events. 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.

We can build up rules of probability, based on an elegantly simple set of axioms called the *axioms of probability*. Let the *sample space* (Ω) be a non-empty set of outcomes and the *event space* ($\mathcal{E}$) be a non-empty set of subsets of Ω. For example, $\Omega = \{1, 2, 3\}$ and one possible *event* is $A = \{1, 3\} \in \mathcal{E}$, where the event is that a 1 or a 3 is observed. The event space $\mathcal{E}$ must satisfy the following properties[1]

1. $A \in \mathcal{E} \quad \Rightarrow \quad A^c \in \mathcal{E}$ (where A^c is the complement of the event A: $A^c = \Omega - A$)
2. $A_1, A_2, \ldots \in \mathcal{E} \quad \Rightarrow \quad \bigcup_{i=1}^{\infty} A_i \in \mathcal{E}$
3. $\mathcal{E}$ is non-empty (in fact, we know from 1 and 2 that $\varnothing \in \mathcal{E}$ and $\Omega \in \mathcal{E}$)

If $\mathcal{E}$ satisfies these three properties, then $(\Omega, \mathcal{E})$ is said to be a *measurable space*. Now we can define the axioms of probability, which make it more clear why these two conditions are needed for our event space to define meaningful probabilities over events. A function $P : \mathcal{E} \to [0, 1]$ satisfies the axioms of probability if

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

is called a *probability measure* or a *probability distribution*. 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 $P(A^c) = 1 - P(A)$. This makes it more clear why we required that if an event is in the event space, then its complement should also be in the event space: if we can measure the probability of an event, then we know that the probability of that event not occurring is 1 minus that probability. Similarly, we require that if two events A_1, A_2 are disjoint, then $P(A_1 \cup A_2) = P(A_1) + P(A_2)$: the probability of either event occurring is the sum of their probabilities, because there is no overlap in the outcomes in the events. Another property

[1] Such a set is usually called a *sigma algebra* or *sigma field*. This terminology feels daunting and is only due to historical naming conventions. Because the sigma algebra is simply the set of events to which we can assign probabilities (measure), we will use the longer but more clear name.

we can infer is that we always have $\Omega, \varnothing \in \mathcal{E}$, where $\varnothing$ corresponds to the event where nothing occurs—which must have zero probability.

Example 1: [Discrete variables (countable)] Consider modeling the probabilities of the roll of a dice. The outcome space is the finite set $\Omega = \{1, 2, 3, 4, 5, 6\}$ and the event space $\mathcal{E}$ is the power set $\mathcal{P}(\Omega) = \{\varnothing, \{1\}, \{2\}, \ldots, \{2, 3, 4, 5, 6\}, \Omega\}$, which consists of all possible subsets of Ω. A natural probability distribution on $(\Omega, \mathcal{E})$ gives each dice roll a 1/6 chance of occurring, defined as $P(\{x\}) = 1/6$ for $x \in \Omega$, $P(\{1, 2\}) = 1/3$ and so on. □

Example 2: [Continuous variables (uncountable)] Consider modeling the probabilities of the stopping time of a car, in the range of 3 seconds to 6 seconds. The outcome space is the continuous interval $\Omega = [3, 6]$. An event could be that the car stops within 3 to 3.1 seconds, giving $A = [3, 3.1] \in \mathcal{E}$. The probability $P(A)$ of such an event is likely low, because it would be a very fast stopping time. We could then start considering all possible time intervals for the event space, and corresponding probabilities. We can already see that this will be a bit more complicated for continuous variables, and so we more rigorously show how to define $\mathcal{E}$ and P below in Section 2.2.2. □

These two examples demonstrate the two most common cases we will encounter: discrete variables and continuous variables. The terms above—countable and uncountable—indicate whether a set can be enumerated or not. For example, the set of natural numbers can be enumerated, and so is countable, whereas the set of real numbers cannot be enumerated—there is always another real number between any two real numbers—and so is uncountable. Though this distinction results in real differences—such as using sums for countable sets and integrals for uncountable sets—the formalism and intuition will largely transfer between the two settings. We will focus mostly on discrete and continuous variables. Much of the same ideas also transfer to mixed variables, where outcome spaces are composed of both discrete and continuous sets such as $\Omega = [0, 1] \cup \{2\}$. Further, for the uncountable setting, we specifically discuss continuous sets, i.e., those are unions of continuous intervals such as $\Omega = [0, 1] \cup [5, 10]$. Because almost all uncountable sets that we will want to consider are continuous, we will interchangeably use the terms continuous and uncountable to designate such spaces. Finally, discrete sets can either be finite, such as $\{1, 2, 3\}$, or countably infinite, such as the natural numbers. Continuous sets are clearly infinite, and are said to be uncountably infinite.

Before going further in-depth on how to define probability distributions, we first introduce *random variables*, and from here on will deal strictly with random variables. A random variable lets us more rigorously define transformations of probability spaces; once we execute that transformation, we can forget about the underlying probability space and can focus on the events and distribution only on the random variable. This is in fact what you do naturally when defining probabilities over variables, without needing to formalize it mathematically. Of course, here we will formalize it.

Consider again the dice example, where now instead you might want to know: what is the probability of seeing a low number (1-3) or a high number (4-6)? We can define a new probability space with $\Omega_X = \{\text{low}, \text{high}\}$, $\mathcal{E}_X = \{\varnothing, \{\text{low}\}, \{\text{high}\}, \Omega_X\}$ and $P_X(\{\text{low}\}) =$

$1/2 = P_X(\{\text{high}\})$. The transformation function $X : \Omega \to \Omega_X$ is defined as

$$X(\omega) \stackrel{\text{def}}{=} \begin{cases} \text{low} & \text{if } \omega \in \{1, 2, 3\} \\ \text{high} & \text{if } \omega \in \{4, 5, 6\} \end{cases}$$

The distribution P_X is immediately determined from this transformation. For example, $P_X(\{\text{low}\}) = P(\{\omega : X(\omega) = \text{low}\})$, because the underlying probability space indicates the likelihood of seeing a $1, 2$ or 3. Now we can answer questions about the probability of seeing a low number of a higher number.

This function X is called a random variable. It is slightly confusing that it is neither random, nor a variable, since X is a function. However, from this point onward, we will treat X like it is a variable that is random, by more simply writing statements like $P_X(X = x)$ or $P_X(X \in A)$, rather than $P(\{\omega : X(\omega) = x\})$ or $P(\{\omega : X(\omega) \in A\})$. For correctness, we can remember that it is a function defined on a more complex underlying probability space. But, in practice, we can start thinking directly in terms of the random variable X and the associated probabilities. Similarly, even for the dice role, we can acknowledge that there is a more complex underlying probability space, defined by the dynamics of the dice. When considering only the probabilities of discrete outcomes from 1-6, we have already implicitly applied a transformation on top of probabilities of the physical system.

Once we have a random variable, it defines a valid probability space $(\Omega_X, \mathcal{E}_X, P_X)$. Therefore, all the same rules of probability apply, the same understanding of how to define distributions, etc. In fact, we can always define a random variable X that corresponds to no transformation, to obtain the original probability space. For this reason, we can move forward assuming we are always dealing with random variables, without losing any generality. We will drop the subscripts, and consider $(\Omega, \mathcal{E}, P)$ to be defined for X. For a more in-depth discussion on random variables, see Appendix **??**.

2.2 Defining distributions

Now we would like to know how to specify P to satisfy the axioms of probability, to model the probability of X taking values in an event A, $P(X \in A)$ with outcome space Ω. This task feels daunting, because it seems we need to define the likelihood for every possible event—set of outcomes—and, in such a way that satisfies the axioms of probability, no less! Fortunately, instead we can define the distribution using a function defined directly on instances $x \in \Omega$. It is convenient to separately consider discrete (countable) and continuous (uncountable) sample spaces. For the discrete case, we will define probability mass functions and for the continuous case, we will define probability density functions.

2.2.1 Probability mass functions

Let Ω be a discrete sample space and $\mathcal{E} = \mathcal{P}(\Omega)$, the power set of Ω. 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 $A \in \mathcal{E}$ is defined as

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

It is straightforward to verify that P satisfies the axioms of probability and, thus, is a probability distribution. For discrete random variables, therefore, we will often write $P(X = x)$, which means that $P(X = x) = p(x)$ for each outcome $x \in \Omega$. We rarely, if ever, define the distribution directly, and rather define the pmf p which induces the distribution P.

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

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

Notice that the distribution P is defined on the elements of $\mathcal{E}$, 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. □

To specify P, therefore, we need to determine how to specify the pmf, i.e., the probability of each discrete outcome. The pmf is often specified as a table of probability values. For example, to model the probability of a birthday for each day in the year, one could have a table of 365 values between zero and one, as long as the probabilities sum to 1. These probabilities could be computed from data about individuals birthdays, using counts for each day and normalizing by the total number of people in the population to estimate the probability of seeing a birthday on a given day. Such a table of values is very flexible, allowing precise probability values to be specified for each outcome. There are, however, a few useful pmfs that have a (more restricted) functional form.

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 $\alpha \in [0, 1]$ 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 the 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 $p(\omega) = \alpha^{\omega}(1 - \alpha)^{1-\omega}$ for $\omega \in \Omega$. The Bernoulli distribution is often written Bernoulli(α). As we will see, a common setting where we use the Bernoulli is for binary classification, say where we try to predict whether a patient has the flu (outcome 0) or does not have the flue (outcome 1).

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

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

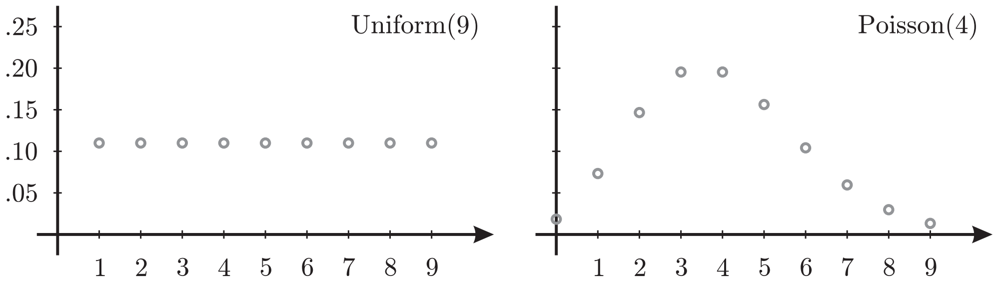


Figure 2.1: Two probability mass functions, for discrete random variables. The Poisson distribution continues further on the x-axis (for variable $\omega \in \mathbb{N}$), with probability decreasing to zero as $\omega \to \infty$.

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.

The *Poisson distribution* reflects the probability of how many incidences occur (implicitly within a fixed time interval). For example, a call center is likely to receive 50 calls per hour, with a much smaller probability on only receiving 5 calls or receiving as many as 1000 calls. This can be modeled with a Poisson(λ), where λ represents the expected number of calls. More formally, $\Omega = \{0, 1, \ldots\}$ and for $\forall \omega \in \Omega$

$$p(\omega) = \frac{\lambda^\omega e^{-\lambda}}{\omega!}.$$

This mass function is hill-shaped, where the top of the hill is mostly centered around λ and there is a skew to having a short, steep left side of the hill and a long, less-steep right tail to the hill. The Poisson distribution is defined over an infinite sample space, but still countable. This is depicted in Figure 2.1.

Exercise 1: Prove that $\sum_{\omega \in \mathbb{N}} p(\omega) = 1$ for the Poisson distribution. □

Example 4: As a prelude to estimating parameters to distributions, consider an example of how we might use a Bernoulli distribution and determine the parameter α to the Bernoulli. A canonical example for Bernoulli distributions is a coin flip, where the outcomes are heads (H) or tails (T). $P(X = \text{H}) = \alpha$ is the probability of seeing H and $P(X = \text{T}) = 1 - \alpha$ is the probability of seeing T. We commonly assume $\alpha = 0.5$; this is called a fair (unbiased) coin. If we flipped the coin many times, we would expect to see about the same number of H and T. However, a *biased* coin may have some skew towards H or T. If we flipped the coin many times, if $\alpha > 0.5$ we should eventually notice more H come up and if $\alpha < 0.5$, we should notice more T.

How might we actually determine this α? An intuitive idea is to use repeated experiments (data), just as described above: flip the coin many times to see if you can gauge the skew. If you see 1000 H and 50 T, a natural guess for the bias is $\alpha = \frac{1000}{1000+50} \approx 0.95$. How confident are you in this solution? Is it definitely 0.95? And how do we more formally define why this should be the solution? This is in fact a reasonable solution, and corresponds to the maximum likelihood solution, as we will discuss in Chapter 5. □

2.2.2 Probability density functions

The treatment of continuous probability spaces is analogous to that of discrete spaces, with probability density functions (pdfs) replacing probability mass functions and integrals replacing sums. In defining pdfs, however, we will not be able to use tables of values, and will be restricted to functional forms. The main reason for this difference stems from the fact that it no longer makes sense to measure the probability of a singleton event. Consider again the stopping time for a car, discussed in Example 2. It would not make a lot of sense to ask the probability of the car stopping in exactly 3.14159625 seconds; realistically, the probability of such a precise event is vanishingly small. In fact, the probability of seeing precisely that stopping time is zero, because the set $\{3.14159625\}$ as a subset of $[3, 6]$ is a set of measure zero. Essentially, it takes up zero mass inside the interval $[3, 6]$, which is after all uncountably infinite. Instead, we will have to consider the probabilities of intervals, like $[4, 5]$ or $[5.667, 5.668]$.

For continuous spaces, we will assume that the set of events $\mathcal{E}$ consists of all possible intervals, called the Borel field $\mathcal{B}(\Omega)$. For example, if $\Omega = \mathbb{R}$, the Borel field $\mathcal{B}(\mathbb{R})$ consists of all open intervals (e.g., $(0, 1)$), closed intervals (e.g.,$[0, 1]$) and semi-open intervals (e.g., $[0, 1)$) in $\mathbb{R}$, as well as sets that can be obtained by a countable number of basic set operations on them, such as unions. This results in a more restricted set of events than the power set of Ω, which would, for example, include sets with only a singleton event. $\mathcal{B}(\mathbb{R})$ is still a huge set—an uncountably infinite set—but still smaller than $\mathcal{P}(\mathbb{R})$. Nicely, though, $\mathcal{B}(\mathbb{R})$ still contains all sets we could conceivably want to measure. The Borel field can be defined for any measurable space, such as higher-dimensional spaces like $\Omega = \mathbb{R}^2$, with events such as $A = [0, 1] \times [0, 1] \subset \Omega$ or $A = [1, 2] \times [-1, 4] \cup [0, 0.1] \times [10, 1000]$.

Let now Ω be a continuous sample space and $\mathcal{E} = \mathcal{B}(\Omega)$. A function $p : \Omega \to [0, \infty)$ is called a *probability density function* (pdf) if[2]

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

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

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

Notice that the definition of the pdf is not restricted to having a range $[0, 1]$, but rather to $[0, \infty)$. For pmfs, the probability of a singleton event $\{\omega\}$ is the value of the pmf at the sample point ω; i.e., $P(\{\omega\}) = p(\omega)$. Since probability distributions P are restricted to the range $[0, 1]$, this implies pmfs must also be restricted to that range. In contrast, the value of a pdf at point ω is not a probability; it can actually be greater than 1. Though it is common when speaking informally to call $p(x)$ the probability of x, more accurately we call this the density at x because it is most definitely not a probability. In fact, as mentioned above, the probability at any single point is 0 (i.e., a countable subset of Ω is a set of measure zero).

A natural confusion is how p can integrate to 1, but actually have values larger than 1. The reason for this is that $p(x)$ can be (much) larger than 1, as long as its only for a very

[2]For correctness, we would like to note that this definition uses Lebesgue integration. You do not need to know about nuanced differences in integration formulations; for all settings we consider, all the definitions are equivalent and your knowledge of integration rules will be effective.

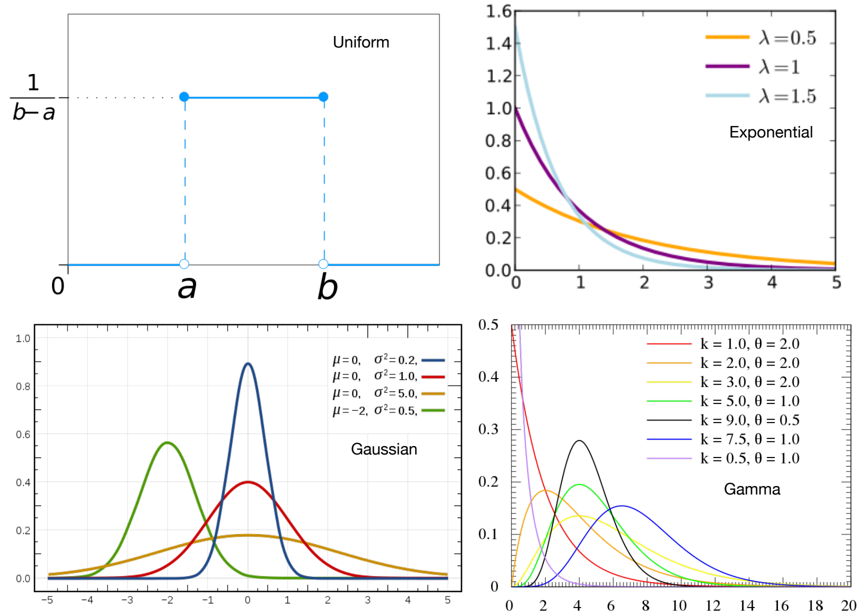


Figure 2.2: Four probability density functions, for continuous random variables. Images taken from Wikipedia.[3]

small interval. Consider the small interval $A = [x, x + \Delta x]$, with probability

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

A potentially large value of the density function is compensated for by the small interval Δx to result in a number between 0 and 1. So, even if $p(x)$ is a million, and the density of points in the small interval or ball around x is large, the probability of an event must still be ≤ 1. The density does indicate that there is high likelihood around that point. By having a huge density around x, this suggests that the density for other points is zero or near zero and that the pdf is extremely peaked around x.

Unlike pmfs, we cannot so easily define pdfs p to flexibly provide specific probabilities for each outcome with a table of probabilities. Rather, for pdfs, we will usually use a known pdf that satisfies the required properties. Further, unlike the discrete case, we will never write $P(X = x)$, because that would be zero. Rather, we will typically write $P(X \in A)$ or more explicitly probabilistic questions like $P(X \leq 5)$. We highlight four pdfs here, that will be used throughout this book; for more examples of pdfs, see Appendix **??**.

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

[3] Many images in this document are currently taken from other sources. This is generally not a good practice, and we will be replacing these images someday soon. We want to highlight that we do not encourage this for formal documents, but only use them here in these educational notes for your benefit temporarily.

$\forall \omega \in [a, b]$ is defined as

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

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 the *support* of the density function.

The *exponential distribution* is defined over a set of non-negative numbers; i.e., $\Omega = [0, \infty)$. For parameter $\lambda > 0$, its pdf is

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

As the name suggests, this pdf has an exponential form, with sharply decreasing probability for values x as they increase in magnitude. 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 $\Omega = \mathbb{R}$, with two parameters, $\mu \in \mathbb{R}$ and $\sigma > 0$ and pdf

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

As we will discuss next, for a random variable that is Gaussian distributed, the parameter μ is the mean or expected value and σ^2 is the variance. We will refer to this distribution as Gaussian(μ, σ^2) or $\mathcal{N}(\mu, \sigma^2)$. When the mean is zero, and the variance is 1 (unit variance), this Gaussian is called the *standard normal.* This specific Gaussian has a name because it is so frequently used. Both Gaussian and exponential distributions are members of a broader family of distributions called the *natural exponential family.*

The *Laplace distribution* is similar to the Gaussian, but is more peaked around the mean. It is also defined over $\Omega = \mathbb{R}$, with two parameters, $\mu \in \mathbb{R}$ and $b > 0$ and pdf

$$p(\omega) = \frac{1}{2b} e^{-\frac{1}{b}|\omega-\mu|}$$

The *gamma distribution* is used to model waiting times, and is similar to the Poisson distribution but for continuous variables. It is defined over $\Omega = (0, \infty)$, with shape parameter $\alpha > 0$ and rate parameter $\beta > 0$ and pdf

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

where $\Gamma(\alpha)$ is called the gamma function. A random variable that is gamma-distributed is denoted $X \sim$ Gamma(α, β).

Example 5: Consider selecting a number (x) between 0 and 1 uniformly randomly (Figure 2.3). What is the probability that the number is greater than or equal to $\frac{3}{4}$ or less than and equal to $\frac{1}{4}$?

Figure 2.3: Selection of a random number (x) from the unit interval $[0, 1]$.

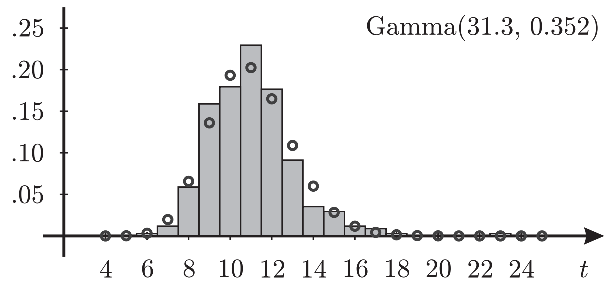


Figure 2.4: A histogram of recordings of the commute time (in minutes) to work. The data set contains 340 measurements collected over one year, for a distance of roughly 3.1 miles. The data was modeled using a gamma family of probability distributions, with the particular location and scale parameters estimated from the raw data. The values of the gamma distribution are shown as dark circles.

We know that $\Omega = [0, 1]$. The distribution is defined by the uniform pdf, $p(\omega) = \frac{1}{b-a} = 1$ where $a = 0, b = 1$ define the interval for the outcome space. We define the event of interest as $A = \left[0, \frac{1}{4}\right] \cup [\frac{3}{4}, 1]$ and calculate its probability as

$$\begin{aligned} P(A) &= \int_0^{1/4} p(\omega) d\omega + \int_{3/4}^{1} p(\omega) d\omega && \triangleright\ p(\omega) = 1 \\ &= \left(\frac{1}{4} - 0\right) + \left(1 - \frac{3}{4}\right) \\ &= \frac{1}{2}. \end{aligned}$$

What if we had instead asked the probability that the number is *strictly greater* than $\frac{3}{4}$ or *strictly less* than $\frac{1}{4}$? Because the probability of any individual event in the continuous case is 0, there is no difference in integration if we consider open or closed intervals. Therefore, the probability would still be $\frac{1}{2}$. □

Example 6: Let's imagine you have collected your commute times for the year[4], and would like to model the probability of your commute time to help you can make predictions about your commute time tomorrow. For this setting, your random variable X corresponds to the commute time, and you need to define probabilities for this random variable. This data could be considered to be discrete, taking values, in minutes, $\{4, 5, 6, \ldots, 26\}$. You could then create histograms of this data (table of probability values), as shown in Figure 2.4, to reflect the likelihood of commute times.

[4]as co-author Predrag amazingly did, and you get to see his fascinating data here.

The commute time, however, is not actually discrete, and so you would like to model it as a continuous RV. One reasonable choice is a gamma distribution. How, though, does one take the recorded data and determine the parameters α, β to the gamma distribution? Estimating these parameters is actually quite straightforward, though not as immediately obvious as estimating tables of probability values; we discuss how to do so in Chapter 5. The learned gamma distribution is also depicted in Figure 2.4.

Given the gamma distribution, one could now ask the question: what is the most likely commute time today? This corresponds to $\max_\omega p(\omega)$, which is called the *mode* of the distribution. Another natural question is the average or expected commute time. To obtain this, you need the expected value (mean) of this gamma distribution, which we define below in Section 2.4. □

2.3 Multivariate random variables

Much of the above development extends to multivariate random variables—a vector of random variables—because the definition of outcome spaces and probabilities is general. The examples so far, however, have dealt with scalar random variables, because for multivariate random variables, we need to understand how variables interact. In this section, we discuss several new notions that only arise when there are multiple random variables, including joint distributions, conditional distributions, marginals and dependence between variables.

Let us start with a simpler example, with two discrete random variables X and Y with outcome spaces $\mathcal{X}$ and $\mathcal{Y}$. There is a joint probability mass function $p : \mathcal{X} \times \mathcal{Y} \to [0, 1]$, and corresponding joint probability distribution P, such that

$$p(x, y) \stackrel{\text{def}}{=} P(X = x, Y = y)$$

where the pmf needs to satisfy

$$\sum_{x\in\mathcal{X}} \sum_{y\in\mathcal{Y}} p(x, y) = 1.$$

For example, if $\mathcal{X} = \{\text{young}, \text{old}\}$ and $\mathcal{Y} = \{\text{no arthritis}, \text{arthritis}\}$, then the pmf could be the table of joint probabilities This fits within the definition of probability spaces, because

		Y = 0	Y = 1
X	0	$P(X{=}0, Y{=}0) = 1/2$	$P(X{=}0, Y{=}1) = 1/100$
	1	$P(X{=}1, Y{=}0) = 1/10$	$P(X{=}1, Y{=}1) = 39/100$

Table 2.1: A joint probability table for random variables X and Y.

$\Omega = \mathcal{X} \times \mathcal{Y}$ is a valid space, and $\sum_{\omega\in\Omega} p(\omega) = \sum_{(x,y)\in\Omega} p(x, y) = \sum_{x\in\mathcal{X}} \sum_{y\in\mathcal{Y}} p(x, y)$. The random variable $Z = (X, Y)$ is a multivariate random variable, of two dimensions.

We can see that the two random variables interact, by looking at the joint probabilities in the table. For example, the joint probability is small for young and having arthritis. Further, there seems to be more magnitude in the rows corresponding to young, suggesting that the probabilities are influenced by the proportion of people in the population that are old or young. In fact, one might ask if we can figure out this proportion just from this table.

The answer is a resounding yes, and leads us to marginal distributions and why we might care about marginal distributions. Given a joint distribution over random variables, one would hope that we could extract more specific probabilities, like the distribution over just one of those variables, which is called the *marginal distribution*. The marginal can be simply computed, by summing up over all values of the other variable

$$P(X = \text{young}) = p(\text{young}, \text{no arthritis}) + p(\text{young}, \text{arthritis}) = \tfrac{51}{100}.$$

A young person either does or does not have arthritis, so summing up over these two possible cases factors out that variable. Therefore, using data collected for random variable $Z = (X, Y)$, we can determine the proportion of the population that is young and the proportion that is old.

In general, we can consider d-dimensional random variable $\boldsymbol{X} = (X_1, X_2, \ldots, X_d)$ with vector-valued outcomes $\boldsymbol{x} = (x_1, x_2, \ldots, x_d)$, such that each x_i is chosen from some $\mathcal{X}_i$. Then, for the discrete case, any function $p : \mathcal{X}_1 \times \mathcal{X}_2 \times \ldots \times \mathcal{X}_d \to [0, 1]$ is called a multidimensional probability mass function if

$$\sum_{x_1 \in \mathcal{X}_1} \sum_{x_2 \in \mathcal{X}_2} \cdots \sum_{x_d \in \mathcal{X} d} p\left(x_1, x_2, \ldots, x_d\right) = 1.$$

or, for the continuous case, $p : \mathcal{X}_1 \times \mathcal{X}_2 \times \ldots \times \mathcal{X}_d \to [0, \infty]$ is a multidimensional probability density function if

$$\int_{\mathcal{X}_1} \int_{\mathcal{X}_2} \cdots \int_{\mathcal{X} d} p\left(x_1, x_2, \ldots, x_d\right) dx_1 dx_2 \ldots dx_d = 1.$$

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. For the discrete case, the marginal distribution $p\left(x_i\right)$ is defined as

$$p\left(x_i\right) \stackrel{\text{def}}{=} \sum_{x_1 \in \mathcal{X}_1} \cdots \sum_{x_{i-1} \in \mathcal{X}_{i-1}} \sum_{x_{i+1} \in \mathcal{X}_{i+1}} \cdots \sum_{x_d \in \mathcal{X}_d} p\left(x_1, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_d\right),$$

where the variable x_i is fixed to some value and we sum over all possible values of the other variables. Similarly, for the continuous case, the marginal distribution $p\left(x_i\right)$ is defined as

$$p\left(x_i\right) \stackrel{\text{def}}{=} \int_{\mathcal{X}_1} \cdots \int_{\mathcal{X}_{i-1}} \int_{\mathcal{X}_{i+1}} \cdots \int_{\mathcal{X}_d} p\left(x_1, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_d\right) dx_1 \ldots dx_{i-1} dx_{i+1} \ldots dx_d.$$

Notice that we use p to define the density over $\boldsymbol{x}$, but then we overload this terminology and also use p for the density only over x_i. To be more precise, we should define two separate functions (pdfs), say $p_{\boldsymbol{x}}$ for the density over the multivariate random variable and p_{x_i} for the marginal. It is common, however, to simply use p, and infer the random variable from context. In most cases, it is clear; if it is not, we will explicitly highlight the pdfs with additional subscripts.

2.3.1 Conditional distributions

Conditional probabilities define probabilities of a random variable X, given information about the value of another random variable Y. More formally, the conditional probability

$p(y|x)$ for two random variables X and Y is defined as

$$p(y|x) \overset{\text{def}}{=} \frac{p(x, y)}{p(x)} \tag{2.1}$$

where $p(x) > 0$.

Exercise 2: Verify that $p(y|x)$ sums (integrates) to 1 over all values $y \in \mathcal{Y}$ for a fixed given $x \in \mathcal{X}$, and thus satisfies the conditions of a probability mass (density) function. □

Equation (2.1) 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

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

By a recursive application of the product rule, we obtain

$$\begin{aligned} p(x_1, \ldots, x_d) &= p(x_d|x_1, \ldots, x_{d-1})p(x_1, \ldots, x_{d-1}) \\ &= p(x_d|x_1, \ldots, x_{d-1})p(x_{d-1}|x_1, \ldots, x_{d-2})p(x_1, \ldots, x_{d-2}) \\ &\vdots \\ &= p(x_d|x_1, \ldots, x_{d-1})p(x_{d-1}|x_1, \ldots, x_{d-2}) \ldots p(x_2|x_1)p(x_1). \end{aligned}$$

More compactly,

$$p(x_1, \ldots, x_d) = p(x_1) \prod_{i=2}^{d} p(x_i|x_1, \ldots, x_{i-1}) \tag{2.2}$$

which is referred to as the *chain rule* or *general product rule*. For example, for three variables, the product rule gives

$$p(x_1, x_2, x_3) = p(x_3|x_2, x_1)p(x_2|x_1)p(x_1)$$

We can also derive *Bayes' rule*, using the product rule:

$$p(x|y) = \frac{p(y|x)p(x)}{p(y)}. \tag{2.3}$$

This uses the fact that giving $p(x, y) = p(x|y)p(y) = p(y|x)p(x)$. Therefore, one really only needs to remember the product rule, to easily recall Bayes' rule.

You may notice that the order of variables in the product rule did not seem to matter. It is in fact somewhat interesting that we can either define the conditional distribution $p(x|y)$ and marginal $p(y)$ or we can define $p(y|x)$ and p(x) and both equivalently recover the joint distribution $p(x, y)$. This property is simply a fact of the definition of conditional distributions, and provides flexibility when estimating distributions. We will most use this equivalence in the form of Bayes rule, when doing parameter estimation and maximum likelihood. For work in graphical models, which is not discussed here, this flexibility is of even greater importance.

2.3.2 Independence of random variables

Two random variables are *independent* if their joint probability distribution factors into the product of the marginals

$$p(x, y) = p(x)p(y).$$

One intuitive reason for this definition can be seen by considering X conditioned on Y. If $p(x|y) = p(x)$, then this means that the value of Y has no influence on the distribution over X, and so they are independent. From the product rule, we know $p(x, y) = p(x|y)p(y)$ and since $p(x|y) = p(x)$, this gives $p(x, y) = p(x)p(y)$ as defined above.

The notion of independence can be generalized to more than two random variables. More generally, d random variables are said to be *mutually independent* or *jointly independent* if a joint probability distribution of any subset of variables can be expressed as a product of marginal probability distributions of its components

$$p(x_1, x_2, \dots, x_d) = p(x_1)p(x_2)\dots p(x_d).$$

Another form of independence, called *conditional independence*, is used even more frequently in machine learning. It represents independence between variables in the presence of some other random variable (evidence); e.g.,

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

Interestingly, the two forms of independence are unrelated: neither one implies the other. X and Y can be independent, but not conditionally independent given Z. X and Y can be conditionally independent given Z, but not independent. We show this in two simple examples in Figure **??** in the Appendix.

Here, we provide an example more directly related to machine learning, about why we care about independence and conditional independence. If two variables are independent, this has important modeling implications. For example, if feature X and target Y are independent, then X is not useful for predicting Y and so is not a useful feature. If two variables are conditionally independent given another variable, this can also have important modeling implications. For example, if we have two features X_1 and X_2, with target Y, where X_2 and Y are conditionally independent given X_1, then feature X_2 is redundant and could potentially be discarded.

As a concrete example, let X_1 = temperature in Celcius and X_2 = temperature in Fahrenheit, with Y = plants need watering. Y is definitely not independent of X_2; however, once X_1 is known (or given), then there is no additional information to be gained from X_2 and so $p(y|x_1, x_2) = p(y|x_1) = p(y|x_2)$. In general, recognizing independencies and conditional independencies can inform and simplify the modeling procedure, and we will see several examples in terms of simplifying maximum likelihood for i.i.d. data and in naive Bayes for classification. We end this section with one more example, using a biased coin, to highlight the distinction between independence and conditional independence.

Example 7: [Biased coin and conditional independence] Assume a manufacturer has produced a biased coin, where it does not equally randomly give heads (H) or tails (T). Rather, it actually has some unknown probability α of seeing H when flipping the coin. Because this bias is unknown, we will encode our uncertainty by defining a random Z = bias of the coin.

In general, this random variable can take values in $[0, 1]$. For the purposes of this example, let's make this a bit simpler, and assume that we know the bias is one of $\mathcal{Z} = \{0.1, 0.5, 0.8\}$. If the bias is 0.5, that would mean this is an unbiased (fair) coin. Let's further assume that we think the probability of each bias is equally likely, meaning $P(Z = z) = 1/3$, because the manufacturer gave us no reason to think any of 0.1, 0.5 or 0.8 to be more likely.

Now imagine that you flip the coin twice, and record the two outcomes x_1 and x_2. These two separate flips correspond to two random variables, X_1 and X_2. The outcome space for X_1 and X_2 is $\{\mathrm{H}, \mathrm{T}\}$. Given the true bias of the coin, α, the true distribution is Bernoulli $P(X_i = \mathrm{H}|Z = \alpha) = \alpha$. However, we do not know the bias α. Instead, we are modeling it with a random variable Z, so that for each given $Z = z$, we know that $P(X_i|Z = z) = z$, i.e., X_i is a Bernoulli random variable with parameter z. Because we do not know the true bias, we have to marginalize over Z to get the marginal distribution over X_1,

$$\begin{aligned}
P(X_1 = x) &= \sum_{z \in \mathcal{Z}} P(X_1 = x, Z = z) \\
&= \sum_{z \in \mathcal{Z}} P(X_1 = x|Z = z)P(Z = z) && \triangleright \text{ product rule} \\
&= P(X_1 = x|Z = 0.1)P(Z = 0.1) + P(X_1 = x|Z = 0.5)P(Z = 0.5)+ \\
&\quad + P(X_1 = x|Z = 0.8)P(Z = 0.8)
\end{aligned}$$

Are X_1 and X_2 conditionally independent given Z? The answer is yes, because given the bias of the coin, knowing the outcome of X_2 does not influence the distribution over X_1, i.e.,

$$P(X_1 = x_1, X_2 = x_2|Z = z) = P(X_1 = x_1|Z = z)P(X_2 = x_2|Z = z)$$

Regardless of what we observe for X_2, we know the distribution over X_1 is a Bernoulli with the given bias z.

Are X_1 and X_2 independent? The answer is no, because without knowing the bias of the coin, knowing the outcome of X_2 tells us something about the Bernoulli distribution over X_1. For example, if $X_1 = \mathrm{T}$ and $X_2 = \mathrm{H}$, then the second outcome suggests that the bias might not be totally skewed towards T. More formally,

$$\begin{aligned}
P(X_1 = x_1, X_2 = x_2) &= \sum_{z \in \mathcal{Z}} P(X_1 = x_1, X_2 = x_2|Z = z)P(Z = z) \\
&= \sum_{z \in \mathcal{Z}} P(X_1 = x_1|Z = z)P(X_2 = x_2|Z = z)P(Z = z)
\end{aligned}$$

which is not guaranteed to equal $P(X_1 = x_1)P(X_2 = x_2)$, where

$$\begin{aligned}
&P(X_1 = x_1)P(X_2 = x_2) \\
&\quad = \left(\sum_{z_1 \in \mathcal{Z}} P(X_1 = x_1|Z = z_1)P(Z = z_1)\right)\left(\sum_{z_2 \in \mathcal{Z}} P(X_2 = x_2|Z = z_2)P(Z = z_2)\right)
\end{aligned}$$

□

2.4 Expectations and moments

The *expected value*, or *mean*, of a random variable X is the average of repeatedly sampled x, in the limit of sampling. It is not necessarily the value we expect to see most frequently—that is called the mode. More precisely, given the pmf or pdf p for outcome space $\mathcal{X}$, the expectation of X is

$$\mathbb{E}[X] \stackrel{\text{def}}{=} \begin{cases} \sum_{x\in\mathcal{X}} xp(x) & \text{if } X \text{ is discrete} \\ \\ \int_{\mathcal{X}} xp(x)dx & \text{if } X \text{ is continuous} \end{cases}$$

For a dice roll, where each number from 1 to 6 has uniform probability, the expected value is 3.5 and the mode is tied for all numbers (i.e., it is multi-modal). For a Bernoulli distribution, where $\mathcal{X} = \{0, 1\}$, the expected value is α, which is not even an outcome that will be observed, but is the average of 0s and 1s if we flipped the coin infinitely many times. The mode in this case depends on α: if $\alpha > 0.5$, making 1 have higher probability, then the mode is 1; if $\alpha < 0.5$, the mode is 0; otherwise, it is bimodal with modes 0 and 1. For a Gaussian distribution, the expected value is the parameter μ, and the mode also equals μ.

In general, we may be interested in the expected value of functions of the random variable X. For example, we may want to know $\mathbb{E}[X^2]$, or more generally $\mathbb{E}\left[X^k\right]$ for some $k > 1$. Or, we may want to know $\mathbb{E}\left[(X - c)^k\right]$ for some $k > 1$ and a constant c. These are called the *moments* of X. In general, for a function $f : \mathcal{X} \to \mathbb{R}$, we can consider $f(X)$ to be a transformed random variables and define its expectation as

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

If $\mathbb{E}[f(X)] = \pm\infty$, we say that the expectation does not exist or is not well-defined.

One useful moment is the *variance*: the central second moment, where central indicates $c = \mathbb{E}[X]$. The variance indicates the amount that the random variable varies around its mean. For example, for a Gaussian distribution, if the variance σ^2 is large, then the Gaussian is very wide, indicating a non-negligible density for a broader range of points x around μ. Alternatively, if σ^2 is almost zero, then the Gaussian is concentrated tightly around μ.

We can also consider conditional expectations, and expectations for multivariate random variables. For two random variables X and Y and function $f : \mathcal{Y} \to \mathbb{R}$, the conditional expectation is

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

Using the identity function $f(y) = y$ results in the standard conditional expectation $\mathbb{E}[Y|x]$.

Exercise 3: Show the *law of total expectations*: $\mathbb{E}[Y] = \mathbb{E}[\mathbb{E}[Y|X]]$, where the outer expectation is over X and the inner expectation is over Y. For example, if both Y and X

are discrete

$$\mathbb{E}[\mathbb{E}[Y|X]] = \sum_{x\in\mathcal{X}} p(x)\mathbb{E}[Y|X=x]$$
$$= \sum_{x\in\mathcal{X}} p(x) \sum_{y\in\mathcal{Y}} yp(y|x)$$

□

For two random variables X and Y and $f : \mathcal{X}\times\mathcal{Y} \to \mathbb{R}$, we can also define the expectation over the joint distribution, with one variable fixed

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

or over both variables

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

For example, if X is continuous and Y is discrete, this gives

$$\mathbb{E}\left[f(X,Y)\right] = \sum_{y\in\mathcal{Y}} p(y)\mathbb{E}\left[f(X,y)\right]$$
$$= \sum_{y\in\mathcal{Y}} p(y) \int_{\mathcal{X}} f(x,y)p(x|y)dx$$

Exercise 4: Show that $\int_{\mathcal{X}} \left(\sum_{y\in\mathcal{Y}} f(x,y)p(x,y)\right) dx = \int_{\mathcal{X}} \mathbb{E}[f(x,Y)]p(x)dx$. □

Just as above with variance, the *covariance* is one important instance of these expected values, with $f(x,y) = (x-\mathbb{E}[X])(y-\mathbb{E}[Y])$. The expected value under this function indicates how the two variables vary together. We use specific notation for the covariance, because it is so frequently used

$$\text{Cov}[X,Y] = \mathbb{E}\left[(X - \mathbb{E}\left[X\right])\left(Y - \mathbb{E}\left[Y\right]\right)\right]$$
$$= \mathbb{E}\left[XY\right] - \mathbb{E}\left[X\right]\mathbb{E}\left[Y\right],$$

with $\text{Cov}[X,X] = V[X]$ being the variance of the random variable X. The *correlation* is the covariance, normalized by the standard deviation—square root of the variance—of each random variable

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

The covariance can become larger, if X and Y themselves have large variance. The correlation, on the other hand, is guaranteed to be between -1 and 1, and so is an scale-invariant measure of how the variables vary together.

Properties of expectations

Here we review some useful properties of expectations. Consider random variables, X and Y. For a constant $c \in \mathbb{R}$, it holds that:

1. $\mathbb{E}[cX] = c\mathbb{E}[X]$
2. $\mathbb{E}[X + Y] = \mathbb{E}[X] + \mathbb{E}[Y]$ ▷ linearity of expectation
3. $\text{Var}[c] = 0$ ▷ the variance of a constant is zero
4. $\text{Var}[X] \stackrel{\text{def}}{=} \text{Cov}[X, X] \succeq 0$, where $\text{Var}[X] \geq 0$ is a scalar. We use $\text{Var}[X]$ as a shorthand for $\text{Cov}[X, X]$.
5. $\text{Var}[cX] = c^2\text{Var}[X]$.
6. $\text{Cov}[X, Y] = \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}(Y)] = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]$
7. $\text{Var}[X + Y] = \text{Var}[X] + \text{Var}[Y] + 2\text{Cov}[X, Y]$ ▷ when $d = m$

In addition, if X and Y are independent random variables, it holds that:

8. $\mathbb{E}[XY] = \mathbb{E}[X]\mathbb{E}[Y]$ for all i, j
9. $\text{Var}[X + Y] = \text{Var}[X] + \text{Var}[Y]$
10. $\text{Cov}[X, Y] = 0$.

Chapter 3

An Introduction to Estimation

We first investigate a simple estimator—a sample average—with a focus on how we can have confidence in our estimate. The sample average is the average of n samples from a distribution. The sample average provides an estimate of the true mean. Depending on the distribution, we might need a larger n to get an accurate estimate. In this chapter, we provide the tools to understand the quality of our sample average, and introduce the concepts of bias, consistency, sample complexity and concentration inequalities.

3.1 Estimating the Expected Value

We assume that we get n samples from an unknown distribution p, over outcome space $\mathcal{X}$. More formally, we assume we have n random variables $X_1, \ldots, X_n$, where $\mathbb{E}[X_i] = \mu$ for some unknown mean μ. The sample average estimator is

$$\bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i \tag{3.1}$$

Intuitively, we know as n gets larger, $\bar{X}$ should get closer and closer to μ. But, how do we show this? We will use concentration inequalities, which gives us the strong law of large numbers, to show this in the next section.

First, let's ask one slightly easier question: is this estimator *unbiased*? The bias of an estimator is how far the expected value of the estimator deviates from the true value. For the sample average estimator, the bias is

$$\text{Bias}(\bar{X}) = \mathbb{E}[\bar{X}] - \mu \tag{3.2}$$

because μ is the true value we are trying to estimate. The estimator is said to be *unbiased* if the Bias is zero. The expectation $\mathbb{E}[\bar{X}]$ reflects that $\bar{X}$ is random, due to the fact that we could have observed many different plausible set of n samples. For example, consider the flips of a coin, with $p(Y = 1) = 0.5$. Imagine the sequence $x_1 = 0, x_2 = 0, x_3 = 1$ was observed, for $n = 3$. The sample average estimator is 1/3. But, another possible sequence could $x_1 = 1, x_2 = 0, x_3 = 1$ with sample average 2/3. The random variable X_1 represents that the first flip could be 0 or 1, with probability 0.5; the random variable X_2 represents that the second flip could be 0 or 1, with probability 0.5; and so on. Because $\bar{X}$ is the average of n random variables, it itself is also random.

Now, let us compute this expectation.

$$\begin{aligned}
\mathbb{E}[\bar{X}] &= \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n} X_i\right] \\
&= \frac{1}{n}\sum_{i=1}^{n} \mathbb{E}\left[X_i\right] && \triangleright\ \mathbb{E}\left[X_i\right] = \mu,\ \text{by assumption} \\
&= \frac{1}{n}\sum_{i=1}^{n} \mu = \frac{1}{n} n\mu \\
&= \mu
\end{aligned}$$

So the bias is zero, because $\text{Bias}(\bar{X}) = \mathbb{E}[\bar{X}] - \mu = \mu - \mu = 0$.

We can also characterize the variance of the estimator. If the X_i are i.i.d. random variables with variance σ^2, then

$$\begin{aligned}
\text{Var}\left[\bar{X}\right] = \text{Var}\left[\frac{1}{n}\sum_{i=1}^{n} X_i\right] &= \frac{1}{n^2}\text{Var}\left[\sum_{i=1}^{n} X_i\right] \\
&= \frac{1}{n^2}\sum_{i=1}^{n} \text{Var}\left[X_i\right] && \triangleright\ \text{by independence} \\
&= \frac{1}{n^2}\sum_{i=1}^{n} \sigma^2 = \frac{1}{n}\sigma^2.
\end{aligned}$$

Therefore, the variance shrinks proportionally to the number of samples. However, this does not give us enough information about how close $\bar{X}$ is to the true mean μ. For this, we use concentration inequalities in the next section.

You might wonder why we care about the bias and variance of our estimator. One reason is simply that once we start thinking about our sample average estimator as a random variable, it is useful to know statistics about the random variable, like its expectation and variance. Another reason is that it helps us reason about the expected mean-squared error of our estimator, as we discuss in Section 3.5.

3.2 Concentration inequalities

Our goal is to obtain a confidence interval around our estimate, to obtain a measure of confidence in our estimate, and to show consistency. More specifically, we would likely be able to say that for any $\epsilon > 0$, there exists $\delta \geq 0$ such that

$$\Pr\left(\left|\bar{X} - \mathbb{E}[\bar{X}]\right| \geq \epsilon\right) \leq \delta. \tag{3.3}$$

In other words, we want a small probability δ that $\bar{X}$ deviates by ϵ from the mean $\mathbb{E}[\bar{X}]$. We want the interval given by ϵ to be small—and of course δ to be small—so that we can be confident in our estimate $\mathbb{E}[\bar{X}]$. This probability tells us that $\mathbb{E}[\bar{X}] \in [\bar{X} - \epsilon, \bar{X} + \epsilon]$ with high probability, that is with probability $1 - \delta$. You can see this is the case by noticing that Equation (3.3) can equivalently be written $\Pr\left(\left|\bar{X} - \mathbb{E}[\bar{X}]\right| \leq \epsilon\right) \geq 1 - \delta$ because

$\Pr\left(\left|\bar{X} - \mathbb{E}[\bar{X}]\right| \le \epsilon\right) = 1 - \Pr\left(\left|\bar{X} - \mathbb{E}[\bar{X}]\right| \ge \epsilon\right)$ and that

$$\begin{aligned}\left|\bar{X} - \mathbb{E}[\bar{X}]\right| \ge \epsilon &\implies -\epsilon \le \mathbb{E}[\bar{X}] - \bar{X} \le \epsilon \\ &\implies \bar{X} - \epsilon \le \mathbb{E}[\bar{X}] \le \bar{X} + \epsilon \qquad \triangleright \text{ Added } \bar{X} \text{ to all three equations.}\end{aligned}$$

Concentration inequalities let us characterize δ for any given ϵ, or ϵ for a given δ. We will discuss two common concentration inequalities: Hoeffding's inequality and Chebyshev's inequality. The second applies to more general settings. Let's start with Hoeffding's inequality. Assume we have independent and identically distributed (i.i.d.) bounded random variables $X_1, \dots, X_n$, such that $a \le X_i \le b$ for some $a, b \in \mathbb{R}$. Then Hoeffding's inequality states that for any $\epsilon > 0$

$$\Pr(|\bar{X} - \mathbb{E}[\bar{X}]| \ge \epsilon) \le 2\exp\left(-\frac{2n\epsilon^2}{(b-a)^2}\right).$$

For a given ϵ, we have $\delta = 2\exp(-2n\epsilon^2/(b-a)^2)$. In many cases, we would actually like to determine the interval around $\mathbb{E}[\bar{X}]$, for some confidence level δ. We can solve for ϵ in terms of δ, to get

$$\delta = 2\exp(-2n\epsilon^2/(b-a)^2) \qquad \implies \epsilon = (b-a)\sqrt{\frac{\ln(2/\delta)}{2n}}.$$

We get that with probability $1-\delta$, $\left|\bar{X} - \mathbb{E}[\bar{X}]\right| \le \epsilon = (b-a)\sqrt{\frac{\ln(2/\delta)}{2n}}$.

Example 8: Let's assume you have n i.i.d. random variables, with $a = 0$ and $b = 1$. Imagine you get $n = 30$ samples, with $\bar{X} = 0.6$. Now you want to get a 95% confidence interval around the true mean, i.e., $\delta = 0.05$. Then the resulting interval, using Hoeffding's inequality, has $\epsilon = (1-0)\sqrt{\frac{\ln(2/0.05)}{2\times 30}} = 0.248$. □

Hoeffding's inequality assumes bounded random variables, but there are other concentration inequalities for unbounded random variables. *Chebyshev's inequality* let's us say that, for i.i.d. random variables $X_1, \dots, X_n$ with variance σ^2,

$$\Pr(|\bar{X} - \mathbb{E}[\bar{X}]| \ge \epsilon) \le \frac{\sigma^2}{n\epsilon^2}. \tag{3.4}$$

Again, we can solve for ϵ in terms of δ, to get

$$\delta = \frac{\sigma^2}{n\epsilon^2} \qquad \implies \epsilon = \sqrt{\frac{\sigma^2}{\delta n}}.$$

For this setting, where we know the variance by the variables are not bounded between some a and b, we still get an interval proportional to $\sqrt{1/n}$. Notice that the conditions for Chebyshev's inequality are actually less stringent, because the variance of any random variable bounded between $[a, b]$ is at most $\sigma^2 = \frac{1}{12}(b-a)^2$. So, Chebyshev's can be applied to such random variables, by using this upper bound on the variance. However, Hoeffding's bound is a better choice, since it gives a tighter bound.

3.3 Consistency

Chebyshev's inequality let's us easily show *consistency* of the sample average estimator. Consistency means that

$$\bar{X} \to \mu \quad \text{as } n \to \infty. \tag{3.5}$$

As n gets larger, $\epsilon = \sqrt{\frac{\sigma^2}{\delta n}}$ gets smaller and smaller. In fact,

$$\sqrt{\frac{\sigma^2}{\delta n}} \to 0 \quad \text{as } n \to \infty. \tag{3.6}$$

This means that for arbitrarily small δ, $\bar{X} \to \mathbb{E}[\bar{X}]$ as $n \to \infty$. Because the sample average is unbiased, we know $\mathbb{E}[\bar{X}] = \mu$, and so $\bar{X} \to \mu$. This convergence in probability is also called the (weak) *law of large numbers*.

3.4 Rate of Convergence and Sample Complexity

The sample complexity n is the number of samples needed to obtain an ϵ accurate estimate. Our goal is to make the sample complexity small, so that we can get a good estimate with as few samples as possible—to be data efficient. The sample complexity is determined both by the properties of the data and by our estimator. We can improve the sample complexity by using smarter estimators, but will inherently have higher sample complexity for certain types of data. For example, if the data has high variance, the bound above tells us that we need more samples to obtain an accurate estimate. But, we can reduce the sample complexity if we could bias or initialize our sample average estimate to be closer to the true mean.

The convergence rate indicates how quickly the error in our estimate decays, in terms of the number of samples. For example, using Chebyshev's inequality, we obtained a convergence rate of $O(1/\sqrt{n})$:

$$\left|\bar{X} - \mathbb{E}[\bar{X}]\right| \leq \sqrt{\frac{\sigma^2}{\delta n}} \quad \text{with high probability } 1 - \delta.$$

This concentration inequality—Chebyshev's inequality—makes few assumptions about the random variables. For example, it does not make any distributional assumptions about each X_i. We can actually reduce the sample complexity, by making stronger assumptions on the X_i.

To see why, let's revisit Equation (3.3), but now assume that the X_i are i.i.d. Gaussian random variables, with variance σ^2 and unknown mean μ. We know that $\bar{X} - \mu$ is zero-mean Gaussian with variance σ^2/n. We can look at the tails of the Gaussian to determine that, say for $\delta = 0.05$, $\epsilon = 1.96\sigma/\sqrt{n}$

$$\Pr(|\bar{X} - \mu| \geq 1.96\sigma/\sqrt{n}) = 0.95$$

Chebyshev's inequality would give a larger number of $\epsilon = 4.47\sigma/\sqrt{n}$. This is 2.28x larger than if we knew the distribution of the X_i were Gaussian, showing what we lose when we do not know the distribution and so cannot take advantage of that information to improve the confidence interval.

Notice that though sample complexity is better, the convergence rate is still $O(1/\sqrt{n})$. Does this mean we are always stuck with this rate? For many distributions, yes, but for certain distributions, we can actually get even faster convergence. For example, for independent Bernoulli X_i, the Chernoff bound—yes, yet another concentration inequality—let's us obtain a convergence rate of $O(1/n)$, which is significantly faster.

3.5 Mean-Squared Error and Bias-Variance

In the above treatment, we assumed our estimator was unbiased. But, we do not actually have to require that our estimator be unbiased. Rather, our ultimate goal is to get an estimator Y for the true mean μ, that is as close to this true value as possible. In some cases, a biased estimator might actually be closer to μ, than an unbiased one.

To see why, let's characterize the squared distance between our estimator Y and μ: $(Y - \mu)^2$. Because Y is random, this difference is random. So instead we can ask: what is the expected squared error of our estimator Y, across all possible datasets?

$$
\begin{aligned}
&\mathbb{E}[(Y-\mu)^2] \\
&= \mathbb{E}[(Y - \mathbb{E}[Y] + \mathbb{E}[Y] - \mu)^2] && \triangleright \text{ Let } b = \text{Bias}(Y) = \mathbb{E}[Y] - \mu \\
&= \mathbb{E}[\big((Y - \mathbb{E}[Y]) + b\big)^2] \\
&= \mathbb{E}[(Y - \mathbb{E}[Y])^2 + 2b(Y - \mathbb{E}[Y]) + b^2] \\
&= \mathbb{E}[(Y - \mathbb{E}[Y])^2] + \mathbb{E}[2b(Y - \mathbb{E}[Y])] + \mathbb{E}[b^2] && \triangleright \text{ By linearity of expectation} \\
&= \text{Var}[Y] + 2b\mathbb{E}[(Y - \mathbb{E}[Y])] + b^2 && \triangleright \text{ By definition } \text{Var}[Y] = \mathbb{E}[(Y - \mathbb{E}[Y])^2] \\
& && \text{and constants come out of expectations} \\
&= \text{Var}[Y] + 2b(\mathbb{E}[Y] - \mathbb{E}[Y]) + b^2 && \triangleright \text{ By linearity of expectation} \\
&= \text{Var}[Y] + \text{Bias}(Y)^2
\end{aligned}
$$

Therefore the mean squared error (MSE) is composed of the variance of Y and the bias of Y. The estimator is unbiased, then it is simply due to the variance of Y. If the dataset is small, for example, then the variance of Y is likely higher and the expected squared error (the MSE) is high due to insufficient samples. On the other extreme, we can get an estimator that has minimal variance: an estimator that always returns 0. This estimator, though, is clearly biased and so will have a high MSE due to a high bias. There are estimators in-between, and in some cases it can be worth having an estimator with a little bit of bias, to help reduce the variance. We see this in the next example.

Example 9: Let's define a biased estimator, $Y = \frac{1}{n+100}\sum_{i=1}^{n} X_i$. This estimator is biased because

$$
\begin{aligned}
\mathbb{E}[Y] &= \mathbb{E}[\frac{1}{n+100}\sum_{i=1}^{n} X_i] \\
&= \frac{1}{n+100}\sum_{i=1}^{n} \mathbb{E}[X_i] \\
&= \frac{n}{n+100}\mu \neq \mu
\end{aligned}
$$

The variance of this estimator, however, is smaller than the sample average estimator:

$$\begin{aligned}
\text{Var}[Y] &= \text{Var}[\frac{1}{n+100}\sum_{i=1}^{n} X_i] \\
&= \frac{1}{(n+100)^2}\text{Var}[\sum_{i=1}^{n} X_i] && \triangleright\ \text{Var}(cX) = c^2\text{Var}(X) \\
&= \frac{1}{(n+100)^2}\sum_{i=1}^{n}\text{Var}[X_i] && \triangleright\ \text{i.i.d. } X_i \\
&= \frac{n}{(n+100)^2}\sigma^2
\end{aligned}$$

You can interpret this estimator as if it saw 100 samples of zeros, and then starting seeing real data $X_1, X_2, \ldots, X_n$, i.e, $Y = \frac{1}{n+100}[\sum_{i=1}^{1}000 + \sum_{i=1}^{n} X_i]$. It is skewed towards the value zero, which could introduce bias if $\mu \neq 0$. But, it also has lower variance since it effectively saw 100 consistent samples corresponding to zero.

Intuitively, if the true mean μ is near zero, the bias introduced is minimal and we can get significant gains from the variance reduction. If μ is far from zero, we might incur a big penalty for the bias. Assume $\sigma = 1.0$, and $n = 10$. Let's compare the MSE for the sample average estimator $\bar{X}$ and for the estimator Y.

Case 1: $\mu = 0.1$. Then, using the results for the bias and variance of the sample average estimator from Section 3.1 we have

$$\begin{aligned}
\text{MSE}(\bar{X}) &= \mathbb{E}[(\bar{X} - \mu)^2] \\
&= \text{Var}[\bar{X}] + \text{Bias}(\bar{X})^2 && \triangleright\ \text{Bias}(\bar{X}) = 0 \\
&= \text{Var}[\bar{X}] && \triangleright\ \text{Var}(\bar{X}) = \frac{\sigma^2}{n} \\
&= \frac{1}{10} && \triangleright\ \sigma = 1.0,\ n = 10
\end{aligned}$$

$$\begin{aligned}
\text{MSE}(Y) &= \mathbb{E}[(\bar{Y} - \mu)^2] \\
&= \text{Var}[Y] + \text{Bias}(Y)^2 \\
&= \frac{n}{(n+100)^2}\sigma^2 + (\frac{n}{n+100}\mu)^2 \\
&= \frac{10}{(110)^2} + (\frac{10}{110}0.01)^2 \approx 9 \times 10^{-4}
\end{aligned}$$

In this case, where μ is not too far from 0, the MSE of Y is much lower than of the sample average estimator.

Case 2: $\mu = 5$ gives

$$\text{MSE}(\bar{X}) = \text{Var}[\bar{X}] = \frac{1}{10}$$

which is the same because $\bar{X}$ is unbiased so its MSE does not depend on the value of μ, and

$$\begin{aligned}
\text{MSE}(Y) &= \text{Var}[Y] + \text{Bias}(Y)^2 \\
&= \frac{n}{(n+100)^2}\sigma^2 + (\frac{n}{n+100}\mu)^2 \\
&= \frac{10}{(110)^2} + (\frac{10}{110}5)^2 \approx 0.2
\end{aligned}$$

In this case, where μ is far from 0, the MSE of Y is much higher than the sample average estimator. The amount of bias introduced is higher, than the gains we obtained from having a lower variance. □

This example illustrates an important phenomenon in machine learning. We often inject some amount of prior knowledge into our learning systems. That prior knowledge often biases the solution, since it changes the solution but is not based on the actual given data. If that prior knowledge is helpful, it can often help constrain the space—and reduce variance—and so make the MSE smaller, even if some bias is incurred. On the other hand, if that prior knowledge is wrong, then it can incur too much bias. In the example above, the prior knowledge was that the mean was likely close to zero. If that prior assumption is correct, then we can get a good estimator with much less data. If the prior assumption is wrong, though, it can significantly degrade performance.

The above example was all about the small sample setting. Once n gets very big, the bias in Y is washed away.

Exercise 5: Show that Y is consistent. □

Chapter 4

Introduction to Optimization

Much of machine learning deals with learning functions by finding the optimal function according to an objective. For example, one may be interested in finding a function $f : \mathbb{R}^d \to \mathbb{R}$ that minimizes the squared differences to some targets for all the samples: $\sum_{i=1}^{n}(f(\mathbf{x}_i) - y_i)^2$. To find such a function, you need to have a basic grasp of optimization techniques.

In this chapter, we discuss basic optimization tools, for generic smooth objectives. Many of the algorithms in machine learning rely on a simple approach: gradient descent. We first discuss how to minimize objectives using both first and second-order gradient descent. This overview covers only a small part of optimization, but fortunately, many machine learning algorithms are based on these simple optimization approaches.

4.1 The basic optimization problem and stationary points

A basic optimization goal is to select a set of parameters $\mathbf{w} \in \mathbb{R}^d$ to minimize a given objective function $c : \mathbb{R}^d \to \mathbb{R}$

$$\min_{\mathbf{w}\in\mathbb{R}^d} c(\mathbf{w})$$

For example, to obtain the parameters $\mathbf{w}$ for linear regression that minimizes the squared differences, we use $c(\mathbf{w}) = \sum_{i=1}^{n}(\langle \mathbf{x}_i, \mathbf{w}\rangle - y_i)^2$, for dot product

$$\langle \mathbf{x}_i, \mathbf{w}\rangle = \sum_{j=1}^{d} x_{ij} w_j.$$

We use the term objective here, rather than error, since error has an explicit connotation that the function is inaccurate. Later we will see that objectives will include both error terms—indicating how accurately they recreate data—as well as terms the provide other preferences on the function. Combining these terms with the error produces the final objective we would like to minimize. For example, for linear regression, we will optimize a regularized objective, $c(\mathbf{w}) = \sum_{i=1}^{n}(\langle \mathbf{x}_i, \mathbf{w}\rangle - y_i)^2 + w_2^2$ where the second term encodes a preference for smaller coefficients w_2.

The goal then is to find $\mathbf{w}$ that minimizes the objective. The most straightforward, naive solution could be to do a random search: generate random $\mathbf{w}$ and check $c(\mathbf{w})$. If any newly generated $\mathbf{w}_t$ on iteration t outperforms the previous best solution $\mathbf{w}$, in that $c(\mathbf{w}_t) < c(\mathbf{w})$, then we can set $\mathbf{w}_t$ to be the new optimal solution. We will assume that our objectives are continuous, and so can take advantage of this smoothness to design better search strategies. In particular, for smooth functions, we will be able to use gradient descent, which we describe in the next section.

Gradient descent enables us to reach stationary points: points $\mathbf{w}$ where the derivative—also called the gradient—is zero. Consider first the univariate case. The derivative tells us

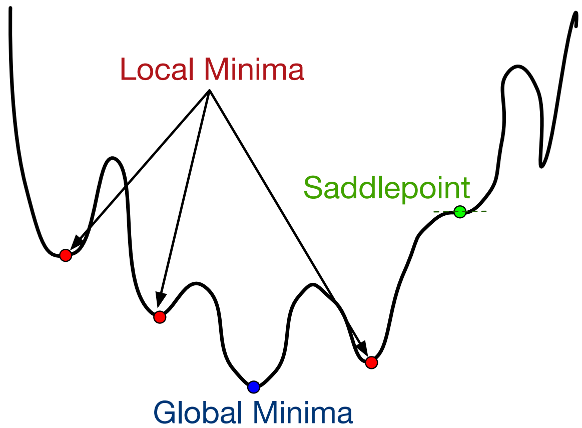


Figure 4.1: Stationary points on a smooth function surface: local minima, global minima and saddlepoints.

the rate of change of the function surface at a point w. When the derivative of the objective is zero at $w \in \mathbb{R}$, i.e., $\frac{d}{dw}c(w) = 0$, this means that locally the function surface is flat. Such points correspond to local minima, local maxima and saddlepoints, as shown in Figure 4.1.

For example, assume again that we are doing linear regression, with only one feature and so only one weight $w \in \mathbb{R}$. The derivative of the objective $c(w) = \sum_{i=1}^{n}(x_i w - y_i)^2$ is

$$\begin{aligned} \frac{d}{dw}c(w) &= \frac{d}{dw}\sum_{i=1}^{n}(x_i w - y_i)^2 \\ &= \sum_{i=1}^{n}\frac{d}{dw}(x_i w - y_i)^2 \\ &= \sum_{i=1}^{n}2(x_i w - y_i)x_i \end{aligned}$$

where the last step follows from the chain rule. Our goal is to find w such that $\frac{d}{dw}c(w) = 0$; once we find such a stationary point, we can then determine if it is a local minimum, local maximum or saddlepoint. Because this objective is convex, we in fact know that all stationary points must be global minima, and so we would not need to do this check. We discuss this further in the last section, where we discuss some properties of objectives.

4.2 Gradient descent

The key idea behind gradient descent is to approximate the function with a Taylor series approximation. This approximation facilitates computation of a descent direction locally on the function surface. We begin by considering the univariate setting, with $w \in \mathbb{R}$. A function $c(w)$ in the neighborhood of point w_0, can be approximated using the Taylor series as

$$c(w) = \sum_{n=0}^{\infty}\frac{c^{(n)}(w_0)}{n!}(w - w_0)^n,$$

where $c^{(n)}(w_0)$ is the n-th derivative of function $c(w)$ evaluated at point w_0. This assumes that $c(w)$ is be infinitely differentiable, but in practice we will take such polynomial approximations for a finite n. A *second-order* approximation to this function uses the first three terms of the series as

$$c(w) \approx \hat{c}(w) = c(w_0) + (w - w_0)c'(w_0) + \frac{1}{2}(w - w_0)^2 c''(w_0).$$

A stationary point of this $\hat{c}(w)$ can be easily found by finding the first derivative and setting it to zero

$$c'(w) \approx c'(w_0) + (w - w_0)c''(w_0) = 0.$$

Solving this equation for w gives us

$$w_1 = w_0 - \frac{c'(w_0)}{c''(w_0)}.$$

Locally, this new w_1 will be an improvement on w_0, and will be a stationary point of this local approximation $\hat{c}$. Moving (far enough) from w_0, however, makes this local second-order Taylor series inaccurate. We would need to check the local approximation at this new point w_1, to determine if we can further improve locally. Therefore, to find the optimal w, we can iteratively apply this procedure

$$w_{t+1} = w_t - \frac{c'(w_t)}{c''(w_t)}. \tag{4.1}$$

constantly improving w_i until we reach a point where the derivative is zero, or nearly zero. This method is called the Newton-Raphson method, or second-order gradient descent.

In first-order gradient descent, the approximation is worse, where we no longer use the second derivative. Instead, when taking a first-order approximation, we know that we are ignoring $O((w - w_0)^2)$ terms, and so the local approximation becomes

$$c(w) \approx \hat{c}(w) = c(w_0) + (w - w_0)c'(w_0) + \frac{1}{2\eta}(w - w_0)^2$$

for some constant $\frac{1}{\eta}$ reflecting the magnitude of the ignored $O((w - w_0)^2)$ terms. The resulting update is then, for step-size η_t

$$w_{t+1} = w_t - \eta_t c'(w_t). \tag{4.2}$$

From this, one can see that, given access to the second derivative, a reasonable choice for the stepsize is $\eta_t = \frac{1}{c''(w_t)}$.

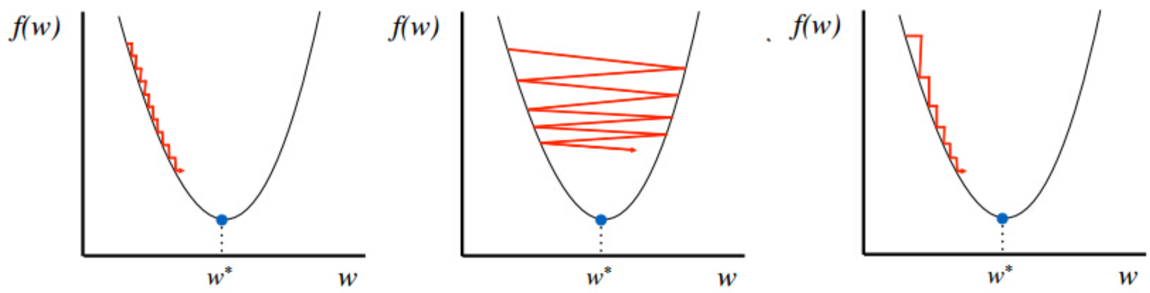
We can similarly obtain such rules for multivariate variables. Gradient descent for $c : \mathbb{R}^d \to \mathbb{R}$ consists of the update

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta_t \nabla c(\mathbf{w}_t). \tag{4.3}$$

where

$$\nabla c(\mathbf{w}_t) = \left(\frac{\partial c}{\partial w_1}(\mathbf{w}_t), \frac{\partial c}{\partial w_2}(\mathbf{w}_t), ..., \frac{\partial c}{\partial w_d}(\mathbf{w}_t) \right) \qquad \in \mathbb{R}^d$$

is the gradient of function c evaluated at $\mathbf{w}_t$. Each *partial derivative* $\frac{\partial c}{\partial w_j}(\mathbf{w}_t)$ indicates how the function c changes if all the variables in $\mathbf{w}_t$ are held constant except for the j element.



(a) Step-size too small (b) Step-size too big (c) Adaptive step-size

Figure 4.2: Different optimization paths, due to different stepsize choices.

As in the single variable setting, the gradient gives a descent direction where stepping (a sufficiently small step) in that direction will decrease the function value. If the gradient is zero, then we are already at a stationary point. We can also similarly derive second-order updates for the multivariate setting, but will only use first-order approaches here with well chosen stepsizes.

4.3 Selecting the step-size

An important part of (first-order) gradient descent is to select the step-size. If the step-size is too small, then many iterations are required to reach a stationary point (Figure 4.2(a)); If the step-size is too large, then you are likely to oscillate around the minimum (Figure 4.2 (b)). What we really want is an adaptive step-size (Figure 4.2 (c)), that likely starts larger and then slowly reduces over time as a stationary point is approached.

The basic method to obtain adaptive step-sizes is to use *line search*. The idea springs from the following goal: we would like to obtain the optimal step-size according to

$$\min_{\eta \in \mathbb{R}^+} c(\mathbf{w}_t - \eta \nabla c(\mathbf{w}_t))$$

The solution to this optimization corresponds to the best scalar stepsize we could select, for the current point $\mathbf{w}_t$ with descent direction $-\nabla c(\mathbf{w}_t)$. Solving this optimization would be too expensive; however, we can find approximate solutions quickly. One natural choice is to use a backtracking line search, that tries the largest reasonable stepsize $\eta_{\max}$, and then reduces it until the objective is decreased. The idea is to search along the line of possible $\eta \in (0, \eta_{\max}]$, with the intuition that a large step is good—as long as it does not overshoot. If it does overshoot, then the stepsize was too large, and should be reduced. The reduction is typically according to the rule $\tau\eta$ for some $\tau \in [0.5, 0.9]$. For $\tau = 0.5$, the stepsize reduces more quickly—halves on each step of the backtracking line search; for $\tau = 0.9$, the search more slowly backtracks from $\eta_{\max}$. As soon as a stepsize is found that decreases the objective, it is accepted. We then obtain a new $\mathbf{w}_t$, again compute the gradient and start the line search once again from $\eta_{\max}$.

This basic line search provides some intuition for our goal in adapting the stepsize. One can, of course, imagine other strategies for selecting the stepsize. We might prefer more efficient choices, even if they are heuristic. For example, for $\mathbf{g}_t \stackrel{\text{def}}{=} \nabla c(\mathbf{w}_t)$ with $g_{t,j}$ the j-th index into $\mathbf{g}_t$, a simple strategy to be robust to big gradients is to use the stepsize $\eta_t = (1 + \sum_{j=1}^{d} |g_{t,j}|)^{-1}$.

Algorithm 1: Line Search($\mathbf{w}_t, c, \mathbf{g} = \nabla c(\mathbf{w}_t)$)

Optimization parameters: $\eta_{\max} = 1.0, \tau = 0.7, \text{tolerance} \leftarrow 10e^{-4}$
$\eta \leftarrow \eta_{\max}$
$\mathbf{w} \leftarrow \mathbf{w}_t$
obj $\leftarrow c(\mathbf{w})$
while number of backtracking iterations is less than maximum iterations **do**
    $\mathbf{w} \leftarrow \mathbf{w}_t - \eta \mathbf{g}$
    // Ensure improvement is at least as much as tolerance
    If $c(\mathbf{w}) <$ obj - tolerance **then break**
    // Else, the objective is worse and so we decrease stepsize
    $\eta \leftarrow \tau\eta$
if maximum number of iterations reached **then**
    // Could not improve solution
    return $\mathbf{w}_t, \eta = 0$
return $\mathbf{w}, \eta$

4.4 Optimization properties

There are several optimization properties to keep in mind when reading this handbook, which we highlight here.

Maximizing versus minimizing We have so far discussed the goal of minimizing an objective. An equivalent alternative is to maximize the negative of this objective.

$$\operatorname*{argmin}_{\mathbf{w} \in \mathbb{R}^d} c(\mathbf{w}) = \operatorname*{argmax}_{\mathbf{w} \in \mathbb{R}^d} -c(\mathbf{w})$$

where argmin returns $\mathbf{w}$ that produces the minimum value of $c(\mathbf{w})$ and argmax returns $\mathbf{w}$ that produces the maximum value of $-c(\mathbf{w})$. The actual min and max values are not the same, since for a given optimal solution, $c(\mathbf{w}) \neq -c(\mathbf{w})$. We opt to formulate each of our optimizations as a minimization, and do gradient descent. It would be equally valid, however, to formulate the optimizations as maximizations, and do gradient ascent.

Convexity A function $c : \mathbb{R}^d \to \mathbb{R}$ is said to be convex if for any $\mathbf{w}_1, \mathbf{w}_2 \in \mathbb{R}^d$ and $t \in [0, 1]$,

$$c(t\mathbf{w}_1 + (1-t)\mathbf{w}_2) \leq tc(\mathbf{w}_1) + (1-t)c(\mathbf{w}_2) \tag{4.4}$$

This definition means that when we draw a line between any two points on the function surface, the function values between these two points all lie below this line. Convexity is an important property, because it means that every stationary point is a global minimum. Therefore, regardless of where we start our gradient descent, with appropriately chosen stepsize and sufficient iterations, we will reach an optimal solution.

A corresponding definition is a concave function, which is precisely the opposite: all points lie above the line. For any convex function c, the negative of that function $-c$ is a concave function.

Uniqueness of the solution We often care if there is more than one solution to our optimization problem. In some cases, we care about *identifiability*, which means we can identify the true solution. If there is more than one solution, one might consider that the problem is not precisely posed. For some problems, it is important or even necessary to have identifiability (e.g., estimating the percentage of people with a disease) whereas for others we simply care about finding a suitable (predictive) function f that reasonably accurately predicts the targets, even if it is not the unique such function. We will not consider identifiability further in this document, but it is important to be cognizant of if your objective has multiple solutions.

Equivalence under a constant shift Adding or multiplying by a constant $a \neq 0$ does not change the solution

$$\operatorname*{argmin}_{\mathbf{w}\in\mathbb{R}^d} c(\mathbf{w}) = \operatorname*{argmin}_{\mathbf{w}\in\mathbb{R}^d} a\ c(\mathbf{w}) = \operatorname*{argmin}_{\mathbf{w}\in\mathbb{R}^d} c(\mathbf{w}) + a.$$

You can see why by taking the gradient of all three objectives and noticing that the gradient is zero under the same conditions

$$\nabla a\ c(\mathbf{w}) = 0 \iff a\nabla c(\mathbf{w}) = 0 \iff \nabla c(\mathbf{w}) = 0$$

and

$$\nabla(c(\mathbf{w}) + a) = 0 \iff \nabla c(\mathbf{w}) = 0.$$

Chapter 5

Formalizing 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 the x_i are i.i.d. from a Gaussian distribution. In this case, the problem of finding the best model can be seen as finding the best parameters μ^* and σ^*: 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 constraints in the parameter space.

5.1 MAP and Maximum Likelihood Estimation

Imagine you observe a dataset of observations $\mathcal{D} = \{x_i\}_{i=1}^n$. The data is drawn from some true distribution p^*, but that distribution is unknown to you. Instead, all you know is that the distribution is in a set of possible distributions, $\mathcal{F}$, sometimes called the *hypothesis space* or function class. For example, $\mathcal{F}$ could be the family of all univariate Gaussian distributions:

$$\mathcal{F} = \{\mathcal{N}(\mu, \sigma^2) \mid \text{ for any } \mu \in \mathbb{R} \text{ and } \sigma \in \mathbb{R}^+\}.$$

The true distribution has parameters μ^* and σ^*; using the data, we would like to find μ and σ as close to these as possible.

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

$$f_{\text{MAP}} = \operatorname*{argmax}_{f \in \mathcal{F}} p(f|\mathcal{D})$$

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. For example, above, we could have equivalently considered $\mathcal{F} = \{(\mu \in \mathbb{R}, \sigma \in \mathbb{R}^+)\}$. We will typically reason directly about the parameter space, or function space, rather than indirectly about the models or probabilities that they parameterize.

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

$$p(f|\mathcal{D}) = \frac{p(\mathcal{D}|f)p(f)}{p(\mathcal{D})}, \tag{5.1}$$

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 over f can be fully described using the likelihood and the prior. Computing this prior, though, can be prohibitively expensive. For example, it could require the estimation of an integral over all possible models f.

Fortunately, finding f_{MAP} can be greatly simplified because $p(\mathcal{D})$ in the denominator does not affect the solution. This is because $p(\mathcal{D})$ is the same regardless of f in the maximization, and so scaling by $p(\mathcal{D})$ does not change the relative ordering

$$\begin{aligned} \max_{f \in \mathcal{F}} \frac{p(\mathcal{D}|f)p(f)}{p(\mathcal{D})} &= \frac{1}{p(\mathcal{D})} \max_{f \in \mathcal{F}} p(\mathcal{D}|f)p(f) \\ \implies \operatorname*{argmax}_{f \in \mathcal{F}} \frac{p(\mathcal{D}|f)p(f)}{p(\mathcal{D})} &= \operatorname*{argmax}_{f \in \mathcal{F}} p(\mathcal{D}|f)p(f). \end{aligned}$$

For this reason, we often write

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

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

$$f_{\text{MAP}} = \operatorname*{argmax}_{f \in \mathcal{F}} p(\mathcal{D}|f)p(f).$$

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, MAP reduces to the maximization of the likelihood function:

$$f_{\text{MLE}} = \operatorname*{argmax}_{f \in \mathcal{F}} p(\mathcal{D}|f).$$

This solution is called the *maximum likelihood* (MLE) 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 is useful to think of MLE as a special case of MAP estimation.

Example 10: 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 a maximum likelihood estimate of λ_0.

The probability mass 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

$$\lambda_{\text{MLE}} = \operatorname*{argmax}_{\lambda \in (0,\infty)} p(\mathcal{D}|\lambda). \tag{5.2}$$

We can write the likelihood function as

$$\begin{aligned} p(\mathcal{D}|\lambda) &= p(\{x_i\}_{i=1}^n |\lambda) \\ &= \prod_{i=1}^n p(x_i|\lambda) \end{aligned}$$

where the probability breaks up into individual probabilities of each x_i because the data is i.i.d. (the random variables are independent). 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 $\ln p(\mathcal{D}|\lambda)$ as

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

because[1]

$$\begin{aligned} \ln p(x_i|\lambda) &= \ln \lambda^{x_i} e^{-\lambda}/(x_i)! \\ &= \ln \lambda^{x_i} + \ln e^{-\lambda} - \ln x_i! \\ &= x_i \ln \lambda - \lambda - \ln x_i!. \end{aligned}$$

[1] Recall that for scalars $a, b > 0$, (i) $\ln(ab) = \ln a + \ln b$ (ii) $\ln(a/b) = \ln a - \ln b$ and (iii) $\ln a^b = b \ln a$

Now in this simpler form, we proceed with computing the derivative

$$\frac{\partial \ln p(\mathcal{D}|\lambda)}{\partial \lambda} = \frac{1}{\lambda}\sum_{i=1}^{n} x_i - n.$$

Solving for λ such that $\frac{\partial \ln p(\mathcal{D}|\lambda)}{\partial \lambda} = 0$ gives us a stationary point of this problem, and we get $\lambda_{\text{MLE}} = \frac{1}{n}\sum_{i=1}^{n} x_i$. We can substitute $n = 6$ and values from $\mathcal{D}$ to compute the solution as

$$\lambda_{\text{MLE}} = \frac{1}{n}\sum_{i=1}^{n} x_i = 5.5$$

which is simply a sample mean.

The second derivative of this log likelihood is always negative because λ must be positive. The second derivative is $-\lambda^{-2}\sum_{i=1}^{n} x_i$ which is < 0 for this λ_{MLE}; 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 (5.2); however, in other situations, we will have to explicitly enforce constraints in the optimization, as we will discuss later.

□

Example 11: 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 with parameters $k = 3$ and $\theta = 1$. Find the MAP estimate of λ_0.

First, we write the probability density function of the gamma distribution for our prior

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

where $\lambda > 0$. $\Gamma(k)$ 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

$$\lambda_{\text{MAP}} = \operatorname*{argmax}_{\lambda \in (0,\infty)} p(\mathcal{D}|\lambda) p(\lambda).$$

As before, we take the log to simplify calculations to get

$$\begin{aligned}
\ln p(\mathcal{D}|\lambda) p(\lambda) &= \ln p(\mathcal{D}|\lambda) + \ln p(\lambda) \\
&= \sum_{i=1}^{n} \ln p(x_i|\lambda) + \ln p(\lambda).
\end{aligned}$$

We have already simplified the first term in the previous example. For the log of the prior distribution, we have

$$\begin{aligned}
\ln p(\lambda) &= \ln\left(\lambda^{k-1} e^{-\frac{\lambda}{\theta}}\right) - \ln(\theta^k \Gamma(k)) \\
&= (k-1)\ln\lambda - \frac{\lambda}{\theta} - \ln(\theta^k \Gamma(k)).
\end{aligned}$$

The last term is constant with respect to λ; so when we take the derivative it will disappear and we will be able to avoid computing it. Plugging everything back in

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

and taking the derivative gives

$$\frac{\partial \ln p(\mathcal{D}|\lambda)p(\lambda)}{\partial\lambda} = \frac{1}{\lambda}\sum_{i=1}^{n} x_i - n + \frac{k-1}{\lambda} - \frac{1}{\theta} \qquad \text{because } \frac{\partial \ln p(\lambda)}{\partial\lambda} = \frac{k-1}{\lambda} - \frac{1}{\theta}$$

Once again setting the derivative to zero and solving for λ gives

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

□

A quick look at λ_{MAP} and λ_{MLE} 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 MLE converge to the same model, f, as long as the prior does not have zero probability (or density) on f. This result shows that the MAP estimate approaches the MLE 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 MLE 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

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

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 MLE 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 [11, Theorem 9.13]).

Example 12: Let $\mathcal{D} = \{x_i\}_{i=1}^{n}$ be an i.i.d. sample from a univariate Gaussian distribution. Our goal is to 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 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

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

and

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

□

MAP and MLE estimates are called *point estimates*. These estimates contrast Bayesian estimates, which estimate the entire posterior distribution or confidence intervals for the parameters, as we discuss in the next section.

5.2 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 or multimodal distributions for the posterior distribution. Bayesian estimation addresses those concerns.

For simplicity in this section, let's assume we are estimating one parameter for a distribution, θ. The main idea in Bayesian statistics is minimization of the *posterior risk*

$$c(\hat{\theta}) = \int_{\mathcal{F}} \text{diff}(\theta, \hat{\theta}) p(\theta|\mathcal{D}) d\theta,$$

where $\hat{\theta}$ is our estimator and $\text{diff}(\theta, \hat{\theta})$ is some difference between two models. When $\text{diff}(\theta, \hat{\theta}) = (\hat{\theta} - \theta)^2$, we can find the $\hat{\theta}$ that minimizes the posterior risk by finding a stationary point, i.e., taking the derivative and setting it to zero

$$\begin{aligned} \frac{\partial}{\partial \hat{\theta}} c(\hat{\theta}) &= 2 \int_{\mathcal{F}} (\hat{\theta} - \theta) p(\theta|\mathcal{D}) d\theta \\ &= 2\hat{\theta} - 2 \int_{\mathcal{F}} \theta \cdot p(\theta|\mathcal{D}) d\theta = 0 \end{aligned}$$

From this, we can see that the optimal minimizer θ_{B}, called the Bayes estimator, is

$$\theta_{\text{B}} = \int_{\mathcal{F}} \theta \cdot p(\theta|\mathcal{D}) d\theta = \mathbb{E}[\theta|\mathcal{D}]$$

This expectation is with respect to the entire posterior distribution $p(\theta|\mathcal{D})$. Bayesian approaches typically require estimation of this posterior. We can compute the posterior, because it can be expressed in terms of known distributions using Bayes rule

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})}.$$

The difficulty, though, is in computing $p(\mathcal{D})$. For MAP, we did not need to estimate $p(\mathcal{D})$ because it was a constant that did not affect finding the most likely parameters. Now, we explicitly need to estimate this term, which we can do using

$$p(\mathcal{D}) = \int p(\mathcal{D}|\theta)p(\theta)d\theta$$

This term, though, is typically much more complex to obtain that either $p(\mathcal{D}|\theta)$ or $p(\theta)$.

In general, computing either the posterior $p(\theta|\mathcal{D})$ or the posterior mean usually involves solving complex integrals. In some situations, these integrals can be solved analytically; in others, numerical integration is necessary. There are classes of distributions for which we know a simple form for the posterior. We discuss this below—with the concept of conjugate priors—but first give an example of computing the Bayes estimator.

Example 13: Let $\mathcal{D} = \{2, 5, 9, 5, 4, 8\}$ yet again be an i.i.d. sample from Poisson(λ_0). Suppose the prior knowledge about the parameter of the distribution can be expressed using a gamma distribution with parameters $k = 3$ and $\theta = 1$. Let's find the posterior distribution and the resulting Bayesian estimate of λ_0, that is $\mathbb{E}[\Lambda|\mathcal{D}]$.

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

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

Though this looks complex, notice that this is actually just a gamma distribution! The parameters k', θ' for this gamma distribution are

$$
\begin{aligned}
k' &= k + \sum_{i=1}^n x_i \\
\theta' &= \frac{\theta}{n\theta+1} = \frac{1}{n+1/\theta}.
\end{aligned}
$$

We know that the expected value of a gamma distribution is $k\theta$, and so we get that

$$
\begin{aligned}
\mathbb{E}[\Lambda|\mathcal{D}] &= \int_0^\infty \lambda p(\lambda|\mathcal{D}) d\lambda = k'\theta' \\
&= \frac{k+\sum_{i=1}^n x_i}{n+\frac{1}{\theta}} \\
&= 5.14
\end{aligned}
$$

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 prior. Such prior distributions are called *conjugate priors*. Conjugate priors simplify the computations in two ways, which are the primary reason for their consideration. First, in many cases it is non-trivial to actually derive $p(\lambda|\mathcal{D})$. Above, we gave you the derivation, but in general it is not easy to explicitly solve for the integral when computing $p(\mathcal{D})$. Second, by knowing the form of the resulting distribution, it is easy to obtain statistics about that distribution. For example, once we knew the posterior was a gamma distribution, it was straightforward to compute the mean. It is similarly straightforward to obtain the mode or median. 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.

Consider if we did not have a conjugate prior. Imagine if instead we chose an exponential distribution as the prior for λ. When computing $p(\mathcal{D})$ and $p(\lambda|\mathcal{D})$, you would simply be stuck with complex integrals and formulas that do not correspond to any known distribution. Instead, if you picked the conjugate prior—the gamma distribution—you simply go look up the known formula for the parameters of the gamma posterior, assuming $p(x|\theta)$ is Poisson and prior $p(\theta)$ is gamma with parameters k and θ. You wouldn't even have to go through the above derivation; you would simply have been able to immediately know that $k' = k + \sum_{i=1}^n x_i$ and $\theta' = \frac{\theta}{n\theta+1}$.

5.3 Maximum likelihood for conditional distributions

We can also formulate MAP and 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 14: 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: $p(x_i, y_i) = p(y_i|x_i)p(x_i)$.

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

Notice that we use $\mu = x_i$ 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

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

□

Exercise 6: We can also formalize this problem as a MAP problem. To do so, we need to pick a prior on the parameter σ. Let's pick a uniform distribution with a relatively narrow range of $[0.5, 2]$. Note that though MLE can be though of as MAP with a uniform prior, this is only the case if we pick a uniform prior that does not restrict the space of feasible solution. This uniform prior, with range $[0.5, 2]$, is quite restrictive, and so we should get a different solution from above. Derive σ^2_{MAP}. □

5.4 [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

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

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

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

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

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

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

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

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 $p(x|\theta_{\text{MLE}}) = p(x|\theta_0)$, if the underlying assumptions are satisfied. Under reasonable conditions, we can infer from it that $\theta_{\text{MLE}} = \theta_0$. 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 6

Introduction to Prediction Problems

Machine learning addresses many problem settings, which can sometimes feel overwhelming. As a non-exhaustive list, these include supervised learning (with classification and regression); semi-supervised learning; unsupervised learning; completion under missing features; structured prediction; learning to rank; statistical relational learning; active learning; and temporal prediction (with time series prediction and policy evaluation in reinforcement learning and online learning). For some of these settings, such as active learning and reinforcement learning, the data collection is a central part of the algorithm and can significantly determine the quality of the learned predictive models. Most other settings assume that data has been collected—without our ability to influence that collection—and now we simply need to analyze that data and learn the best predictors that we can. In this passive setting, we can either assume that the data is i.i.d.—which is the most common—or that there are dependencies between data points—such as in time series prediction or statistical relational learning. There are also settings where the data is incomplete, say because a user did not fill in their age.

One ontology, therefore, could consider the following dimensions to categorize machine learning problems:

1. passive vs. active
2. i.i.d. vs. non-i.i.d.
3. complete vs. incomplete.

As with all ontologies, each problem will not perfectly fit into these categories. Further, it is likely that most data collection is not completely passive (even if only because the human modeler influences collection of data), is likely not i.i.d. (even if we intended it to be), and likely has some missing components. Nonetheless, algorithms will make these assumptions, to varying degrees, even if the data does not satisfy those assumptions. For the majority of these notes, we will focus on the simplest setting: passive, i.i.d. and complete.

In this chapter, we will first introduce classification and regression and then discuss criteria for selecting functions for classification and regression, to motivate the algorithms developed in later chapters.

6.1 Supervised learning problems

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 *input* or *observation* and $y_i \in \mathcal{Y}$ the corresponding target. 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 an *instance*

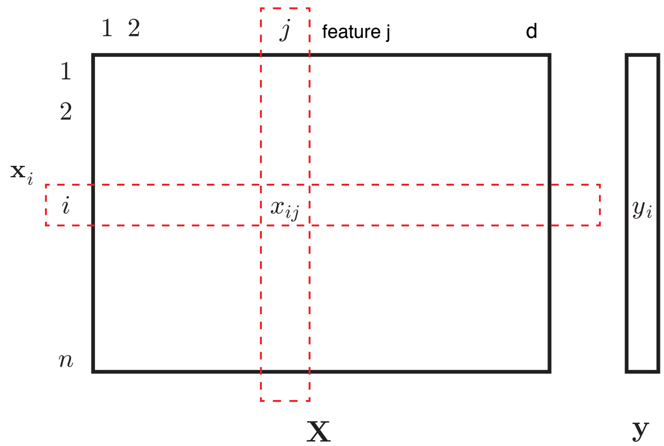


Figure 6.1: Notation for the dataset. **X** *is an n-by-d matrix, with rows corresponding to instances and columns to features. y is an n-by-*1 *vector of targets.*

or a *sample*.[1] Each dimension of x_j is typically called a *feature* or an *attribute*. We will often organize the dataset into a matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ where each row corresponds to a sample $\mathbf{x}_i$ and each column corresponds to a feature (see Figure 6.1).

The distinction between $\mathbf{x}$ and y is due to the fact that we assume that the features are relatively 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 (e.g., presence of a disease or the final selling price of a house before it has sold). 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 observations for which target values have already been collected. In deployment, we can use this model to make predictions from easy-to-obtain information—the observation—about hard-to-obtain information—the targets.

6.1.1 Regression and Classification

The differences in algorithms for prediction problems, with i.i.d. complete data, typically arises from the properties of the inputs (observations) and the properties of the targets. For example, we may need to treat text observations—such as those from a set of documents—differently than a ten-dimensional real-valued observation vector of sensor readings reflecting the temperature and pressure in a physical system. A simple, and relatively common strategy, to handle these differences is to map different types of observations—language, categorical variables and even sequence data—into a Euclidean space where the observation is re-represented as a real-valued vector. Many prediction algorithms are designed for real-valued observations, and so standard algorithms can be applied. This question of data representation is a central problem in machine learning. For this course, we will assume the observations are already in a convenient form, as a d-dimensional real-valued vector.

The properties of the target are also important, and result in two typical distinctions for

[1] In statistics, a sample usually refers to a collection of randomly sampled $\mathbf{x}$, rather than a single instance. It is common in machine learning, though, to use the word sample to mean a single sample, rather than multiple samples or draws from the distribution.

prediction problems: classification and regression. Generally speaking, we have a regression problem when $\mathcal{Y}$ is continuous and a classification problem if $\mathcal{Y}$ is discrete. In **regression** possible target set include $\mathcal{Y} = \mathbb{R}$ or $\mathcal{Y} = [0, \infty)$. An example of a regression problem is shown in Table 6.1.

	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 6.1: 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.

In **classification** we construct a function that predicts discrete class labels; this function is typically called a *classifier*. The cardinality of $\mathcal{Y}$ in classification problems is usually small, e.g. $\mathcal{Y} = \{\text{healthy}, \text{diseased}\}$. An example of a data set for classification with $n = 3$ data points and $d = 5$ features is shown in Table 6.2.

Classification problems can be further subdivided into multi-class and multi-label problems. A multi-class problem consists of providing the single label for an input. For example, for (simple) blood-type with $\mathcal{Y} = \{\text{A}, \text{B}, \text{AB}, \text{O}\}$, a patient can only be labeled with one of these labels. Within multi-class problems, if there are only two classes, it is called binary classification, such as the example in Table 6.2. In multi-label, an input can be associated with more than one label. An example of a multi-label problem is the classification of text documents into categories such as $\{\text{sports}, \text{medicine}, \text{travel}, \text{politics}\}$. Here, a single document may be related to more than one value in the set; e.g. an article on sports medicine. The learned function can now return multiple outputs.

Typically, to make the outputs more consistent between these two settings, the output for both multi-class and multi-label is an indicator vector. For $m = |\mathcal{Y}|$, the prediction for blood types might be [0 1 0 0] to indicate blood-type B and the prediction for four article labels could be [1 1 0 0] if it is both an article pertaining to sports and medicine.

	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 6.2: 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.

6.1.2 Deciding how to formalize the problem

Though we separate supervised learning problems into two categories, it is not always clear cut how a problem should be formalized. For example, consider the output space $\mathcal{Y} = \{0, 1, 2\}$. We can treat this as a multi-class classification problem, or we could presume $\mathcal{Y} = [0, 2]$ and learn a regression model. We can then threshold the predictions returned by the regression model, by rounding them to the closest integer.

How do you decide which problem formulation to use? Though the mathematical procedures in machine learning are precise, deciding how to formulate real-world problem is subtle, and so inherently less clear-cut. 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. In this example, you could ask: is there inherently an ordering to the outputs $\{0, 1, 2\}$? If not, say they correspond to `Prefers apples, Prefers oranges, Prefers bananas`, then it may be a poor choice to model the output as an interval, which often implies ordering. On the other hand, regression functions can be easier to learn and often produce surprisingly good classification predictions. Further, if there is an ordering to these classes, say `Good, Better, Best`, then most classification models— which do not assume an ordering on the outputs—would not be able to take advantage of this ordering to improve prediction performance.

Formalizing the problem and selecting the function class, and objective is an important step in using machine learning effectively. Fortunately, there is a wealth of knowledge, especially empirically, that can guide this selection. As you learn more about the methods, combined with some information about structure in your domain, you will become better at this specification.

6.2 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. To do so, we assume we have access to the true joint distribution $p(\mathbf{x}, y)$ and ask what the optimal prediction would be in this ideal case. The optimal predictor is defined based on a cost function $\mathrm{cost} : \mathcal{Y} \times \mathcal{Y} \to [0, \infty)$, where $\mathrm{cost}(\hat{y}, y)$ reflects the cost or penalty for predicting $\hat{y}$ when the true target is y. Because X, Y are random, the cost $C = \mathrm{cost}(f(X), Y)$ is also a random variable, because it is a function of these random variables. Our goal is to minimize the expected cost. We first consider a few examples of costs, and then derive the optimal predictors.

6.2.1 Examples of Costs

The costs for classification and regression are usually different. A typical cost function for classification is

$$\mathrm{cost}(\hat{y}, y) = \begin{cases} 0 & \text{when } y = \hat{y} \\ \\ 1 & \text{when } y \neq \hat{y} \end{cases} \tag{6.1}$$

A more complex cost function might arise in settings where certain inaccurate predictions are more problematic than others. Let's consider a concrete example, in a 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. Here, the cost is better depicted as a table It is not always possible to define a meaningful cost

		Y	
		-1 (¬Has Disease)	1 (Has Disease)
$\hat{Y}$	-1 (¬Has Disease, No Test)	0	1000
	1 (Has Disease, Do Test)	1	1

Table 6.3: The cost function for the medical lab, cost($\hat{y}, y$), with $c_{\text{lawsuit}} = 1000$ and $c_{\text{lab}} = 1$.

function and, thus, a reasonable criterion is to use the default 0-1 loss in Equation (6.1).

In regression, common costs are the squared error

$$\text{cost}(\hat{y}, y) = (\hat{y} - y)^2 \tag{6.2}$$

and the absolute error

$$\text{cost}(\hat{y}, y) = |\hat{y} - y|. \tag{6.3}$$

The squared error more heavily penalizes values further away from y than the absolute error. There are many other costs, that factor in the magnitude of the targets, such as the percentage error.

6.2.2 Deriving the Optimal Predictors

We begin first by deriving the optimal classifier. We can express the expected cost as follows, assuming the inputs are continuous real-valued vectors and the targets are from a discrete set $\mathcal{Y}$ and $\hat{y} = f(\mathbf{x})$ for the given predictor f

$$\begin{aligned}
\mathbb{E}[C] &= \int_{\mathcal{X}} \sum_{y \in \mathcal{Y}} \text{cost}(f(\mathbf{x}), y) p(\mathbf{x}, y) d\mathbf{x} \\
&= \int_{\mathcal{X}} p(\mathbf{x}) \sum_{y \in \mathcal{Y}} \text{cost}(f(\mathbf{x}), y) p(y|\mathbf{x}) d\mathbf{x},
\end{aligned}$$

where the integration is over the entire input space $\mathcal{X} = \mathbb{R}^d$. Notice that we have to predict one class for each observation: $f(\mathbf{x})$ can only output one value $\hat{y}$ in $\mathcal{Y}$. But, the target is random. Because of this the optimal classifier f^* may not be able to obtain zero cost. However, simply by looking at the above equation, we can obtain $f^* = \text{argmin}\, \mathbb{E}[C]$, by picking the best classifier for each $\mathbf{x}$ separately

$$\begin{aligned}
f^*(\mathbf{x}) &= \underset{\hat{y} \in \mathcal{Y}}{\text{argmin}}\, \mathbb{E}[C|X = \mathbf{x}] \\
&= \underset{\hat{y} \in \mathcal{Y}}{\text{argmin}} \sum_{y \in \mathcal{Y}} \text{cost}(\hat{y}, y) p(y|\mathbf{x}).
\end{aligned}$$

This classifier is called the *Bayes risk classifier*.

If we use the 0-1 cost function, in Equation (6.1), the Bayes risk classifier simply becomes

$$\begin{aligned}
f^*(\mathbf{x}) &= \underset{\hat{y}\in\mathcal{Y}}{\text{argmin}} \sum_{y\in\mathcal{Y}} \text{cost}(\hat{y}, y)p(y|\mathbf{x}) \\
&= \underset{\hat{y}\in\mathcal{Y}}{\text{argmax}} \left(1 - \sum_{y\in\mathcal{Y}} \text{cost}(\hat{y}, y)p(y|\mathbf{x})\right) \\
&= \underset{\hat{y}\in\mathcal{Y}}{\text{argmax}} \sum_{y\in\mathcal{Y}} (1 - \text{cost}(\hat{y}, y))p(y|\mathbf{x}) && \triangleright \text{ because } \sum_{y\in\mathcal{Y}} p(y|\mathbf{x}) = 1 \\
&= \underset{\hat{y}\in\mathcal{Y}}{\text{argmax}} \sum_{y\in\mathcal{Y}, y\neq\hat{y}} 0 \cdot p(y|\mathbf{x}) + \sum_{y\in\mathcal{Y}, y=\hat{y}} 1 \cdot p(y|\mathbf{x}) \\
&= \underset{y\in\mathcal{Y}}{\text{argmax}}\, p(y|\mathbf{x})
\end{aligned}$$

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 similar to 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

$$\mathbb{E}[C] = \int_{\mathcal{X}} \int_{\mathcal{Y}} \text{cost}(f(\mathbf{x}), y)p(\mathbf{x}, y)dyd\mathbf{x}.$$

For simplicity, we will consider the squared error from Equation (7.1)

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

which results in

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

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 finding $\hat{y}$ for each $\mathbf{x}$ to minimize

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

To find the optimal $\hat{y}$, we can solve this minimization problem by finding a stationary point, the global minimum. To do so, we differentiate g with respect to $\hat{y}$ and find the point where the derivative equals zero

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

Therefore, the optimal predictor is

$$f^*(\mathbf{x}) = \mathbb{E}[Y|\mathbf{x}].$$

Therefore, the optimal regression model in the sense of minimizing the square error between the prediction and the true target is the conditional expectation $\mathbb{E}[Y|X = \mathbf{x}]$.[2]

Exercise 7: We can similarly compute the optimal predictor for the absolute error cost, in Equation (6.3). Show that the optimal predictor for the absolute error is the conditional median, $\text{Median}[Y|X = \mathbf{x}]$. □

The above has motivated that learning $p(y|\mathbf{x})$ is sensible for classification, to reduce 0-1 classification error. An alternative to directly learning $p(y|\mathbf{x})$ is to instead learn the class-conditional and prior distributions, $p(\mathbf{x}|y)$ and $p(y)$, respectively. Using

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

we can see that these two learning approaches are equivalent in theory, to decide the $\hat{y}$ with highest $p(y|\mathbf{x})$. 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*.

6.2.3 Reducible and Irreducible Error

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

[2] 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 $\mathbf{x}$.

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

When $f(\mathbf{x}) = \mathbb{E}[Y|\mathbf{x}]$, the expected cost can be simply expressed as

$$\begin{aligned}\mathbb{E}[C] &= \int_{\mathcal{X}} p(\mathbf{x}) \int_{\mathcal{Y}} (\mathbb{E}[Y|\mathbf{x}] - y)^2 p(y|\mathbf{x}) dy d\mathbf{x} \\ &= \int_{\mathcal{X}} p(\mathbf{x}) \text{Var}\left[Y|X = \mathbf{x}\right] d\mathbf{x} \end{aligned} \tag{6.4}$$

Recall that $\text{Var}\left[Y|X = \mathbf{x}\right]$ is the variance of Y, for the given $\mathbf{x}$. The expected cost, therefore, reflects the cost incurred from noise or variability in the targets. This is the best scenario in regression for a squared error cost; we cannot achieve a lower expected 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

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

Notice that the expected value of $g(\mathbf{x}, Y)$ for each $\mathbf{x}$ is zero because

$$\begin{aligned}\mathbb{E}[g(\mathbf{x}, Y)] &= \mathbb{E}\Big[(f(\mathbf{x}) - \mathbb{E}[Y|\mathbf{x}])(\mathbb{E}[Y|\mathbf{x}] - Y)|\mathbf{x}\Big] \\ &= (f(\mathbf{x}) - \mathbb{E}[Y|\mathbf{x}])\mathbb{E}\Big[(\mathbb{E}[Y|\mathbf{x}] - Y)|\mathbf{x}\Big] \\ &= (f(\mathbf{x}) - \mathbb{E}[Y|\mathbf{x}])\left(\mathbb{E}[Y|\mathbf{x}] - \mathbb{E}[Y|\mathbf{x}]\right) \\ &= 0.\end{aligned}$$

Therefore, we can conclude that $\mathbb{E}[g(\boldsymbol{X}, Y)] = 0$, when taking expectations over $\boldsymbol{X}$. We can now express the expected cost as

$$\begin{aligned}\mathbb{E}[C] &= \mathbb{E}[(f(\boldsymbol{X}) - Y)^2] \\ &= \underbrace{\mathbb{E}[(f(\boldsymbol{X}) - \mathbb{E}[Y|\boldsymbol{X}])^2]}_{\text{reducible error}} + \underbrace{\mathbb{E}[(\mathbb{E}[Y|\boldsymbol{X}] - Y)^2]}_{\text{irreducible error}}.\end{aligned}$$

The first term reflects how far the trained model $f(\mathbf{x})$ is from the optimal model $\mathbb{E}[Y|\mathbf{x}]$. The second term reflects the inherent variability in Y given $\mathbf{x}$, as written in Equation (6.4). 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 error is inherent or irreducible in the sense that no matter how much we improve the function, we cannot reduce this term. 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.

Chapter 7

Linear Regression and Polynomial 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 start by hypothesizing the functional form of this relationship. For example, the function f might be a linear function

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

where we need to learn $\mathbf{w} = (w_0, w_1, w_2)$. Alternatively, we might hypothesize that f is a nonlinear function, such as $f(x) = \alpha + \beta x_1 x_2$, where α and β is another set of parameters to be learned.

In this chapter, we focus on estimating linear functions. The function is modeled as a *linear combination* of features and parameters, i.e.

$$f(\mathbf{x}) = w_0 + w_1 x_1 + \dots w_d x_d = \sum_{j=0}^{d} w_j x_j = \mathbf{x}^\top \mathbf{w}$$

where we extended $\mathbf{x}$ to $(x_0 = 1, x_1, x_2, \dots, x_d)$. This extension to the vector is for simplicity of notation: it allows us to write $f(\mathbf{x})$ as a dot product, and avoid having to specially account for the intercept term w_0. Finding the best parameters $\mathbf{w} \in \mathbb{R}^{d+1}$ is referred to as the *linear regression problem.* We begin by formalizing this as a maximum likelihood problem.

7.1 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 input $\boldsymbol{X} = (X_1, X_2, \dots, X_d)$, 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 $\boldsymbol{\omega} = (\omega_0, \omega_1, \dots, \omega_d)$ is a set of unknown coefficients we seek to recover through estimation, and $X_0 = 1$ is the intercept term. Generally, the assumption of normality for the error term is reasonable (recall the central limit theorem!), although the independence between ε and $\boldsymbol{X}$ 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

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

where we use the notation $\exp(a) = e^a$, to make the exponent easier to read. Observe that the only change from the conditional density function of Y is that coefficients $\mathbf{w}$ are used instead of $\boldsymbol{\omega}$. The MLE problem, where we assume the space of possible values for the weights is $\mathcal{F} \subset \mathbb{R}^{d+1}$ is

$$\begin{aligned}
\mathbf{w}_{\text{MLE}} &= \operatorname*{argmin}_{\mathbf{w}\in\mathcal{F}} -\sum_{i=1}^{n} \ln p(y_i|\mathbf{x}_i, \mathbf{w}) \\
&= \operatorname*{argmin}_{\mathbf{w}\in\mathcal{F}} -\sum_{i=1}^{n} \ln \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - \mathbf{x}_i^\top \mathbf{w})^2}{2\sigma^2}\right) \\
&= \operatorname*{argmin}_{\mathbf{w}\in\mathcal{F}} -\sum_{i=1}^{n} \left[-\ln\sqrt{2\pi\sigma^2} - \frac{(y_i - \mathbf{x}_i^\top \mathbf{w})^2}{2\sigma^2}\right] \\
&= \operatorname*{argmin}_{\mathbf{w}\in\mathcal{F}} \sum_{i=1}^{n} \ln\sqrt{2\pi\sigma^2} + \sum_{i=1}^{n} \frac{(y_i - \mathbf{x}_i^\top \mathbf{w})^2}{2\sigma^2} \qquad \triangleright \text{ first term is constant wrt } \mathbf{w} \\
&= \operatorname*{argmin}_{\mathbf{w}\in\mathcal{F}} \sum_{i=1}^{n} \frac{(y_i - \mathbf{x}_i^\top \mathbf{w})^2}{2\sigma^2} \qquad \triangleright \text{ dropping the first term does not change the solution} \\
&= \operatorname*{argmin}_{\mathbf{w}\in\mathcal{F}} \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - \mathbf{x}_i^\top \mathbf{w})^2 \qquad \triangleright \text{ scaling by } 2\sigma^2 \text{ does not change the solution} \\
&= \operatorname*{argmin}_{\mathbf{w}\in\mathcal{F}} \sum_{i=1}^{n} (y_i - \mathbf{x}_i^\top \mathbf{w})^2 \qquad (7.1)
\end{aligned}$$

The resulting objective is intuitive. Our prediction $\hat{y}_i \overset{\text{def}}{=} \mathbf{x}_i^\top \mathbf{w}$. The MLE formulation states that we should find the weights that minimize the squared differences between our predictions $\hat{y}_i$ and the given y_i. A simple example illustrating the linear regression problem is shown in Figure 7.1. In the next sections, we will discuss how to solve this optimization and the properties of the solution.

Note that here it seems obvious that we could have just started with the squared error objective. This is in fact how ordinary least squares (OLS) was originally introduced. However, there are two reasons that we use the MLE approach. First, 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. Second, for other distributions $p(y|\mathbf{x})$—such as the Bernoulli when we do classification—guessing a good objective is much less obvious. For those situations, we will often turn to

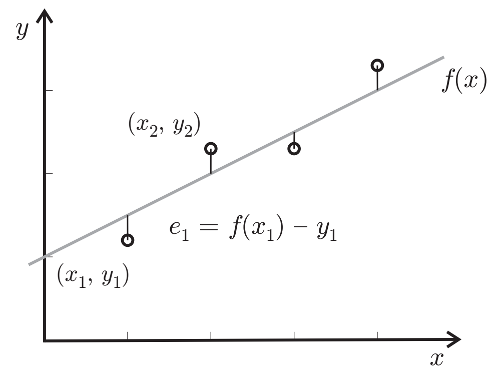


Figure 7.1: A linear regression solution on data set $\mathcal{D} = \{(1, 1.2), (2, 2.3), (3, 2.3), (4, 3.3)\}$. The task of the optimization process is to find the best linear function $f(x) = w_0 + w_1 x$ so that the sum of squared errors $e_1^2 + e_2^2 + e_3^2 + e_4^2$ is minimized.

an MLE formulation to help us define a reasonable objective for our parameters. When possible, it is better to take a more unified approach.

Example 15: Consider again data set $\mathcal{D} = \{(1, 1.2), (2, 2.3), (3, 2.3), (4, 3.3)\}$ from Figure 7.1. We want to find the maximum likelihood coefficients—the least-squares fit—for $f(x) = w_0 + w_1 x$. The problem corresponds to finding the solution with the following variables

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \mathbf{x}_3^\top \\ \mathbf{x}_4^\top \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix}, \ \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}, \ \mathbf{y} = \begin{bmatrix} 1.2 \\ 2.3 \\ 2.3 \\ 3.3 \end{bmatrix},$$

where a column of ones was added to $\mathbf{x}$ to allow for a non-zero intercept w_0. We can substitute $\mathbf{X}$ and $\mathbf{y}$ into Equation (7.3) below, to get the solution $\mathbf{w} = (0.7, 0.63)$. At this point, the gradient w.r.t. $\mathbf{w}$ of the sum of squared errors is zero and the sum of squared errors is 0.223. □

7.2 Linear Regression Solution

To minimize the sum of squared errors, let's define

$$c_i(\mathbf{w}) = (f(\mathbf{x}_i) - y_i)^2 = \tfrac{1}{2}\left(\mathbf{x}_i^\top \mathbf{w} - y_i\right)^2, \tag{7.2}$$

with the full objective as

$$c(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n} c_i(\mathbf{w})$$

We added a normalization by the number of samples, so that we have an average squared error rather than a cumulative error. This optimization is equivalent, since normalization by a fixed constant does not change the solution: $\text{argmin}_{\mathbf{w}} \frac{1}{n}\sum_{i=1}^{n} c_i(\mathbf{w}) = \text{argmin}_{\mathbf{w}} \sum_{i=1}^{n} c_i(\mathbf{w})$. Numerically, though, the average error is more sensible to optimize, since it will not grow with more data. The cumulative error, on the other hand, can get very big if n is big. So, to implement a solution, we will use Equation (7.2) instead of Equation (7.1). Similarly, we used $\frac{1}{2}$ in front of Equation (7.2) without changing the solution; this will be convenient later to cancel the 2 that comes from the gradient.

Notice that to compute the gradient of the objective, it decomposes into a sum of gradients for each sample

$$\nabla c(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n} \nabla c_i(\mathbf{w})$$

and so we simply need to determine the gradient of the error for each sample $(\mathbf{x}_i, y_i)$. We can use the chain rule, by introducing variable $u = \mathbf{x}_i^\top \mathbf{w} - y_i$, to get

$$\begin{aligned}
\frac{\partial c_i(\mathbf{w})}{\partial w_j} &= \frac{\partial \frac{1}{2}(\mathbf{x}_i^\top \mathbf{w} - y_i)^2}{\partial w_j} \\
&= \frac{\partial \frac{1}{2}u^2}{\partial u}\frac{\partial u}{\partial w_j} && \triangleright\ u \stackrel{\text{def}}{=} \mathbf{x}_i^\top \mathbf{w} - y_i \\
&= u\frac{\partial (\sum_{m=0}^{d} x_{im}w_m - y_i)}{\partial w_j} \\
&= u\sum_{m=0}^{d}\frac{\partial x_{im}w_m}{\partial w_j} = u x_{ij} && \triangleright\ \frac{\partial x_{im}w_m}{\partial w_j} = 0 \text{ for } m \neq j \\
&= (\mathbf{x}_i^\top \mathbf{w} - y_i)x_{ij}
\end{aligned}$$

This derivation is for any $0 \leq j \leq d$.

Our goal is to find $\mathbf{w}$ such that $\frac{\partial c(\mathbf{w})}{\partial w_j} = 0$ for all $0 \leq j \leq d$. We obtain a system of equations, with $d+1$ variables and $d+1$ equations

$$\begin{aligned}
\tfrac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i^\top \mathbf{w} - y_i)x_{i0} &= 0 \\
\tfrac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i^\top \mathbf{w} - y_i)x_{i1} &= 0 \\
&\vdots \\
\tfrac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i^\top \mathbf{w} - y_i)x_{id} &= 0
\end{aligned}$$

which can be equivalently written in vector notation as $\frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i^\top \mathbf{w} - y_i)\mathbf{x}_i = \mathbf{0}$, where $\mathbf{0}$ is the $d+1$ vector of all zeros. We can turn to linear algebra to obtain a solution. We can write down the matrix and vector that correspond to this linear system of equations

$$\begin{aligned}
\mathbf{A} &\stackrel{\text{def}}{=} \tfrac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i\mathbf{x}_i^\top \in \mathbb{R}^{(d+1)\times(d+1)} \\
\mathbf{b} &\stackrel{\text{def}}{=} \tfrac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i y_i \in \mathbb{R}^{d+1}
\end{aligned} \tag{7.3}$$

Then our goal is to find $\mathbf{w}$ such that $\mathbf{A}\mathbf{w} = \mathbf{b}$. If $\mathbf{A}$ is invertible, then $\mathbf{w} = \mathbf{A}^{-1}\mathbf{b}$.

In practice, though, it is more common to solve for the weights $\mathbf{w}$ using gradient descent. For gradient descent, we would initialize the weights $\mathbf{w}$ at some random initialization and iteratively update $\mathbf{w}$ until we reach a point where the gradient is approximately. This is shown in the pseudocode, in Algorithm 2.

Algorithm 2: Gradient Descent for a given objective c

Fix iteration parameters: tolerance $= 10^{-4}$ and max iterations $= 10^5$
$\mathbf{w} \leftarrow$ random vector in $\mathbb{R}^d$
err $\leftarrow \infty$
while $|c(\mathbf{w}) - \text{err}| >$ tolerance and have not reached max iterations **do**
  err $\leftarrow c(\mathbf{w})$ ▷ for linear regression, $c(\mathbf{w}) = \frac{1}{2n}\sum_{i=1}^{n}(\mathbf{x}_i^\top \mathbf{w} - y_i)^2$
  $\mathbf{g} \leftarrow \nabla c(\mathbf{w})$ ▷ for linear regression, $\nabla c(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i^\top \mathbf{w} - y_i)\mathbf{x}_i$
  // The step-size η could be chosen by line-search, as in Algorithm 1
  $\eta \leftarrow$ line search$(\mathbf{w}, c, \mathbf{g})$
  $\mathbf{w} \leftarrow \mathbf{w} - \eta\mathbf{g}$
return $\mathbf{w}$

Using gradient descent can be more efficient than solving for $\mathbf{w} = \mathbf{A}^{-1}\mathbf{b}$. Each gradient descent update costs $O(nd)$, whereas the solution to the linear system costs $O(d^3 + d^2n)$. It costs d^2n to construct $\mathbf{A}$ and matrix inversion[1] costs approximately $O(d^3)$. If we use k iterations for gradient descent, then gradient descent costs $O(ndk)$ in total. For big d and fewer samples, gradient descent is almost definitely more efficient. Further, we can get to an approximate solution with gradient descent efficiently, with a relatively small number of iterations.

The cost of gradient descent, though, is still quite high because we have to iterate over the entire dataset to compute the gradient. It is not uncommon to have very large datasets. Rather, what is really used in practice is the much more efficient *stochastic gradient descent*. We describe this in the next section, Section 7.3.

Exercise 8: Show that $\mathbf{A} = \frac{1}{n}\mathbf{X}^\top\mathbf{X}$ and $\mathbf{b} = \frac{1}{n}\mathbf{X}^\top\mathbf{y}$. Further, show that $c(\mathbf{w}) = \frac{1}{n}\|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2$. Note that $\|\mathbf{v}\|_2 = \sqrt{\mathbf{v}^\top\mathbf{v}} = \sqrt{v_1^2 + v_2^2 + \dots v_n^2}$ is the ℓ_2 norm, and $\|\mathbf{v}\|_2^2 = \mathbf{v}^\top\mathbf{v}$ is simply the square of the norm that removes the square-root. □

7.3 Stochastic Gradient Descent and 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 objective function, $\nabla c(\mathbf{w})$. Computing this gradient for a large number of 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, or a small mini-batch of b samples (e.g., $b = 32$). For example, if using one sample to approximate the gradient ($b = 1$), you would randomly sample a

[1] We can actually use other linear system solvers to find $\mathbf{w}$ such that $\mathbf{A}\mathbf{w} = \mathbf{b}$; the best strategy is not necessarily to compute the matrix inverse. But, the costs are still typically close to $O(d^3)$, so for simplicity of analysis we use this computational complexity.

datapoint i and update the weights on iteration t using

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta_t(\mathbf{x}_i^\top \mathbf{w} - y_i)\mathbf{x}_i$$

for some stepsize η_t.

At first glance, this might seem a little crazy. How can we get a good descent direction, with such a rough approximation to the gradient? The true gradient requires summing the gradients for all samples, and we use only one of those gradients! Can we even say anymore that our algorithm will converge? 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]). In fact, with modern dataset sizes that are very large, it is the most common strategy in use in machine learning.

The key idea for why this works is simple: the gradient for a single sample is an unbiased estimate of the true gradient. Notice that the batch gradient can be seen as an expectation where each sample $(\boldsymbol{X}_i, Y_i)$ in the dataset has a uniform probability of $\frac{1}{n}$, for $\boldsymbol{X}_k$ an $d+1$ random vector. In stochastic gradient descent, we sample a random datapoint $(\boldsymbol{X}_k, Y_k)$ uniformly—proportionally to this probability of $\frac{1}{n}$—and so get that

$$\begin{aligned}
\mathbb{E}[(\boldsymbol{X}_k^\top \mathbf{w} - Y_k)\boldsymbol{X}_k] &= \sum_{i=1}^{n} p(i)(\mathbf{x}_i^\top \mathbf{w} - y_i)\mathbf{x}_i \\
&= \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i^\top \mathbf{w} - y_i)\mathbf{x}_i.
\end{aligned}$$

Exercise 9: Show that the mini-batch stochastic gradient is also an unbiased estimate of the batch gradient.

$$\text{Mini-batch Gradient for Linear Regression } = \frac{1}{k}\sum_{k=1}^{b}(\mathbf{x}_{i_k}^\top \mathbf{w} - y_{i_k})\mathbf{x}_{i_k} \tag{7.4}$$

for $i_1, \ldots, i_b$ sampled uniformly from $\{1, \ldots, n\}$. □

This stochastic gradient descent approach is shown in Algorithm 3. Each step corresponds to updating with a randomly chosen mini-batch of data. Typically, in practice, this entails iterating one or more times over the dataset in order (assuming it is random, with i.i.d. samples). Each iteration over the dataset is called an *epoch*. The conditions for convergence typically include conditions on the step-sizes, requiring them to decrease over time. In practice, though, we often use a fixed stepsize η_0, a stepsize that decays with the epoch number, or smarter stepsize algorithms that use statistics on the magnitude of the gradient. For example, similarly to an algorithm called AdaGrad [7], we can normalize the stepsize by the sum of accumulating gradients: $\eta_t = \eta_0(1 + \bar{g}_t)^{-1}$ where $\bar{g}_t = \bar{g}_{t-1} + \frac{1}{d+1}\sum_{j=0}^{d}|g_{t,j}|$. After many epochs, 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.

Algorithm 3: Stochastic Gradient Descent for objective $c(\mathbf{w}) = \frac{1}{n} c_i(\mathbf{w})$

Fix iteration parameters: number of epochs $= 10^4$ and mini-batch size $b = 32$
$\mathbf{w} \leftarrow$ random vector in $\mathbb{R}^d$
for $p = 1, \ldots$ number of epochs **do**
  Shuffle data points from $1, \ldots, n$
  for $k = 1, \ldots, n$ **do**
    $\mathbf{g} \leftarrow \nabla c_k(\mathbf{w})$ ▷ for linear regression, $\nabla c_k(\mathbf{w}) = (\mathbf{x}_k^\top \mathbf{w} - y_k)\mathbf{x}_k$
    // For convergence, the step-size η_t needs to decrease with time, such as $\eta_t = p^{-1}$
    // In practice, it is common to use stepsizes that do not decay with time
    // such as picking a small fixed stepsize ($\eta = 0.01$), or using stepsize adaptation
    $\eta \leftarrow p^{-1}$
    $\mathbf{w} \leftarrow \mathbf{w} - \eta \mathbf{g}$
return $\mathbf{w}$

Remark: In many cases, the dataset is actually constantly growing. Data is constantly being gathered, and new samples are streaming in. In this streaming setting—also called an online setting—stochastic gradient descent allows us to avoid storing all the data, since we simply do updates with the most recent samples. Further, the stochastic gradient update is an unbiased estimate of the gradient of the true expected error, $\mathbb{E}[(\boldsymbol{X}^\top \mathbf{w} - Y)\boldsymbol{X}]$ where the expectation is over all pairs $(\boldsymbol{X}, Y)$. Each new datapoint is a random sample from the joint distribution over $(\boldsymbol{X}, Y)$.

7.4 Polynomial Regression: Using Linear Regression to Learn Non-linear Predictors

At first, it might seem that the applicability of linear regression 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 because we can use it to obtain non-linear functions. The main idea is to apply a non-linear transformation to the observation vector $\mathbf{x}$ prior to the fitting step. A linear function in this new feature space provides a nonlinear function in the original observation space. In this section, we will discuss one such nonlinear transformation: polynomials. Many other nonlinear transformations are possible—see for example radial basis functions, wavelets, and Fourier basis to name a few. The idea, though, is the same, and so we will use polynomials as one representative example.

Let's start by considering one-dimensional data, i.e., $d = 1$. In OLS regression, we would learn the function

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

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

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

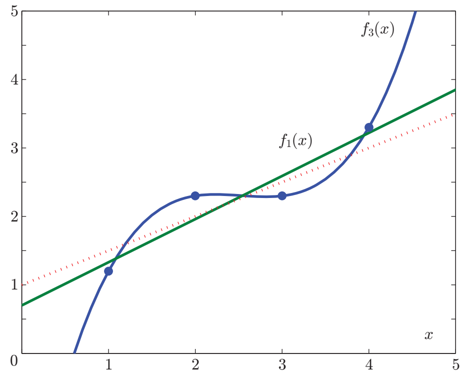


Figure 7.2: Example of a linear vs. polynomial fit on a data set shown in Figure 7.1. The linear fit, $f_1(x)$, is shown as a solid green line, whereas the cubic polynomial fit, $f_3(x)$, is shown as a solid blue line. The dotted red line indicates the target linear concept.

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

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

where $\phi_j(x) = x^j$ and $\boldsymbol{\phi} = (\phi_0(x), \phi_1(x), \ldots, \phi_p(x))$. We simply apply this transformation to every data point x_i to get a new dataset $\{(\phi(x_i), y_i)\}$. Then we use linear regression on this dataset, to get the weights $\mathbf{w}$ and the nonlinear predictor $f(x) = \sum_{j=0}^{p} w_j \phi_j(x)$, which is a polynomial (nonlinear) function in the original observation space.

Example 16: In Figure 7.1 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 by using function $1 + \frac{x}{2}$ and then adding a measurement error $\boldsymbol{\epsilon} = (-0.3, 0.3, -0.2, 0.3)$. It turned out that the optimal coefficients $\mathbf{w}_{\text{MLE}} = (0.7, 0.63)$ 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 $p = 3$.

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 average squared error on the dataset equals $c(\mathbf{w}_2) = 0.055$ and $c(\mathbf{w}_3) \approx 0$. Thus, the best fit is achieved with the cubic polynomial.

Note that this polynomial is strictly more expressive than either the linear function and the degree two polynomial, since it can always choose to set the weights to zero and ignore the added features. It is no surprise, then, that it can achieve a lower squared error than either the linear function or the quadratic function. As we discuss in the next chapter, however, this cubic function is actually not a good predictor. It can achieve a better fit, but does not generalize well to new data nor does it discover the true linear function that generated the data. □

The same idea extends to multivariate observation vector $\mathbf{x}$. Each transformation $\phi_j(\mathbf{x})$ is a non-linear function of the input $\mathbf{x}$. For example, for $\mathbf{x} = (x_1, x_2)$, we could define polynomial basis

$$\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} \phi_0(\mathbf{x}) = 1.0 \\ \phi_1(\mathbf{x}) = x_1 \\ \phi_2(\mathbf{x}) = x_2 \\ \phi_3(\mathbf{x}) = x_1 x_2 \\ \phi_4(\mathbf{x}) = x_1^2 \\ \phi_5(\mathbf{x}) = x_2^2 \end{bmatrix}$$

This transformation allows us to learn a degree-2 polynomial, now with 6 variables $w_0, \ldots, w_5$ to learn rather than the 3 we would learn for $(x_0 = 1, x_1, x_2)$. We can similar obtain a cubic functions, adding the required terms for degree-3 polynomial, including $x_1^2 x_2$, $x_1^2 x_2^2$, x_1^3 and so on. The number of variables for this cubic, if we include all the possible terms, is 10.

In general, for a p-degree polynomial on d inputs, the number of terms corresponds to number of combinations of choosing p elements from a set of $d+1$ elements[2] if repetition is allowed: $\binom{(d+1)+p-1}{p} = \binom{d+p}{p}$. So, for two variables, the quadratic has $\binom{2+2}{2} = \binom{4}{2} = 6$; the cubic has $\binom{2+3}{3} = \binom{5}{3} = 10$; and a quartic would have $\binom{2+4}{4} = \binom{6}{4} = 15$. For three variables, the quadratic has $\binom{3+2}{2} = \binom{5}{2} = 10$; the cubic has $\binom{3+3}{3} = \binom{6}{3} = 20$; and a quartic would have $\binom{3+4}{4} = \binom{7}{4} = 35$.

Remark: Recall that in linear regression, we made the assumption that Y given an input $\mathbf{x}$ is Gaussian distributed: $Y \sim \mathcal{N}(\mu = \mathbf{x}^\top \mathbf{w}, \sigma^2)$. The distribution of the observation vector itself was not relevant. Under this nonlinear transformation, we can similarly notice we are making a Gaussian assumption. However, now the mean for the Gaussian is a more complex, nonlinear function of $\mathbf{x}$: $Y \sim \mathcal{N}(\mu = \boldsymbol{\phi}(\mathbf{x})^\top \mathbf{w}, \sigma^2)$.

[2]It is $d+1$ because in the polynomial input we consider $x_0 = 1.0$ to be a valid term to select.

Chapter 8

Generalization Error and Evaluation of Models

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 models and the algorithms based on a finite sample. Imagine a setting where you learn two models, say using linear regression and polynomial regression. Which of these two models is "better"? What does it even mean to say better? 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 empirical tools to better evaluate the properties of learning algorithms and models. We will start by discussing the idea of generalization error: the error of a model on new data. This reflects how well that model generalizes to data it did not get train on, which reflects our ultimate goal of deploying predictors to make predictions on new data. We will discuss the nuances in trying to accurately estimate this generalization error. 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 or model's 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 scratches the surface of the complex topic of proper evaluation of learning algorithms and models. For a nice overview of evaluation for machine learning algorithms, see [9].

8.1 Generalization Error and Overfitting

Our goal is to minimize generalization error: the expected cost. For a given loss, or cost $\text{cost}(\hat{y}, y)$, the goal is to minimize the expected cost, $\mathbb{E}[C] = \int_{\mathcal{X}\times\mathcal{Y}} p(\mathbf{x}, y)\text{cost}(f(\mathbf{x}), y) d\mathbf{x} dy$. We already saw this goal when talking about optimal predictors. But, we cannot directly minimize the generalization error; instead, we have minimized an empirical error. For example, for regression, we minimized a sample average squared error $\frac{1}{n}\sum_{i=1}^{n}(f(\mathbf{x}_i) - y_i)^2$

which is an unbiased and consistent estimate of the true expected cost. A natural question is, for this minimum $\mathbf{w}$ of the empirical cost on the given training dataset, how well does it do in terms of the expected cost?

One might hope that by minimizing the empirical cost, that we should do well in terms of the expected cost. After all, a sample average is a reasonable estimate of the expectation. Unfortunately, in some cases, minimizing the empirical cost can produce functions that generalize poorly. Consider the following extreme example. Let f be a function that memorizes the data. For every observed $\mathbf{x}_i$, it returns precisely y_i. For any $\mathbf{x}_i$ that are not observed, it returns 0. This function will get zero empirical error—also called training error—but will not generalize at all and is likely to do very poorly in terms of the expected cost—the generalization error.

This effect is called *overfitting*. The term comes from the idea that the function has overly specialized—or overly fit itself—to the training set, at the expense of performing well for other data points. Overfitting typically occurs because the complexity of the model is increased considerably, whereas the size of the data set remains small relative to this model size. Even with modern datasets that are quite large, model complexity has increased at a commiserate pace, and so these very large models overfit to the large datasets.

Example 17: Let's return to the polynomial regression example, shown in Figure 7.2. Now, instead of simply asking how well the function can fit the data, we ask how well it performs on new data. To evaluate the learned models, we generate a testing dataset of 100 samples with observations $x \in \{0, 0.1, 0.2, \ldots, 10\}$ and noise-free target values 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 average error on the training dataset equals $c(\mathbf{w}_2) = 0.05$ and $c(\mathbf{w}_3) \approx 0$. Thus, the best fit is achieved with the cubic polynomial. However, the average error on the test dataset reveals poor generalization ability of the cubic model. The average squared errors are $c_{\text{test}}(\mathbf{w}) = 0.269$, $c_{\text{test}}(\mathbf{w}_2) = 0.039$, and $c_{\text{test}}(\mathbf{w}_3) = 220.185$. It is clear the cubic model is overfitting, which is not surprising considering it has much higher model complexity than the linear models—and higher than is required to actually fit the data. □

Though we know overfitting occurs, it is not always obvious to see that it is occurring. One signature of overfitting is an increase in the magnitude of the coefficients. This manifests in the above 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. (We will discuss *regularization* in Chapter 9 as an approach to prevent this effect.) This occurs because the cubic function has four unknowns (four parameters) and only four observations: it can fit this small dataset of four examples perfectly. In particular, it can fit the noise ϵ in the targets by adding and subtracting large numbers to get the precise y values. For sample $(x = 1, y = 1.2)$, we have $f(x) = -3.1 + 6.6 * 1 - 2.65 * 1^2 + 0.35 * 1^3 = 1.2$. For sample $(x = 2, y = 2.3)$, we have $f(x) = -3.1 + 6.6 * 2 - 2.65 * 2^2 + 0.35 * 2^3 = 2.3$. And so on. The function contorts to an odd solution, so that it can perfectly match the given y, even though we actually know that these may not be optimal—our goal is $\mathbb{E}[Y|x]$.

More generally, we can measure overfitting by obtaining samples of generalization error. If we have an independent dataset, called a test set, we can obtain a sample average estimate of the generalization error. Unlike the training set, this test set gives an unbiased estimate

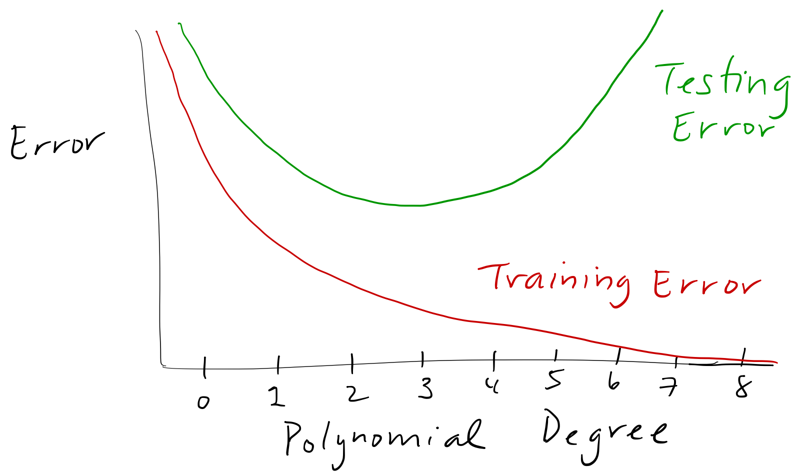


Figure 8.1: Hypothetical training and testing error, for polynomial regression with increasing polynomial degree. The training error decreases with increasing degree (increasing model complexity). The testing error improves, when using more complex models, but then starts to degrade with higher-order polynomials due to overfitting.

of the generalization error because our model was not fit to it. (We discuss more about how to get good estimates of generalization error in Section 8.2.) In general, if there is a significant mismatch between training and testing error, this could indicate overfitting. We cannot simply compare the numbers, because we generally expect training error to be lower than testing error (generalization error). The weights were chosen to minimize that error, after all. A function could be quite good in terms of generalization error, and still have lower training error than testing error. Instead, it is typically easier to gauge overfitting by comparing different models. For example, you could increase model complexity, such as trying all polynomials up to degree p, and then see at what degree the testing error stops decreasing and starts increasing, as in Figure 8.1.

Models may not only suffer from overfitting; they can also suffer from *underfitting*. The problem here is usually that the model class is insufficient to represent the true model, and so is not able to obtain a good fit. In this case, the training error can be quite high. Another way to see this is that the learned model cannot explain the data. It is reasonable to expect that with growing dataset sizes, for increasingly complex problems, our models will begin to suffer more from underfitting than overfitting. The true model—determined by complex interactions in the world—is likely not in our function class.

8.2 Obtaining Samples of Error

The most straightforward way to obtain a measure of the performance—generalization error—for a model is to use a test set, as discussed in the previous section. Before doing any training, a part of the data is set to the side—or held out—to only be used at the very end to gauge performance of our learned function. For example, if we have 10,000 samples, we could use $n = 8000$ for training and $m = 2000$ for testing. Once the function is trained on the n training examples, its performance can be measured on the test. To give an unbiased sample of generalization error, this hold-out test set cannot be used in any way during training.

Once we have these m samples of error, we can try to make statistically sound conclusions about performance. We can use confidence intervals, with the sample average error on the test set, to gauge the level of certainty in this estimate of the generalization error. If our confidence intervals are narrow, then we can be relatively confident in our estimate. If the confidence intervals are quite wide, then we need to exercise caution using our estimate and it might be worthwhile gathering more data for testing before any deployment. Further, we can also use these m estimates of error to compare different models, say one using polynomial regression with $p = 2$ and another with $p = 3$. We discuss using statistical significance tests to make high-probability claims about differences between algorithms, in the next section.

In this course, we will simply assume access to a held-out test set. However, there are more effective strategies to get samples of error; for your interest, a discussion about two others approaches are included here. 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 uses the idea behind bootstrapping: the data itself is a reasonable model of the underlying distribution. Sampling from the data 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.

To better understand the properties of these two approaches, see the thorough and accessible explanation in [8, Chapter 5].

8.3 Making Statistically Significant Claims

Now that we have a mechanism to obtain m (unbiased) samples of error, we can turn to obtaining statistically significant (high-probability) claims about the performance of models. Suppose we have m samples, and wish to compare learned functions f_1 and f_2. When measuring performance on these m samples, we find that f_1 seems to perform better on average than f_2. But can we say that it is actually better? In this section, we discuss this questions, that is how to claim that f_1 is better than f_2, with high-probability, or realize that we cannot make such claims.

8.3.1 Computing Confidence Intervals Tests

One of the easiest approaches for evaluating and comparing models is to use a tool we already know: confidence intervals. We can compute a sample average error for a learned function f, using the m samples of error from the test set: $\bar{X} = \frac{1}{m}\sum_{i=1}^{m} c_i(f)$ where $c_i(f)$ is the error for the ith sample. For example, we could have a learned linear function $f(\mathbf{x}) = \mathbf{x}^\top \mathbf{w}$ and a squared error $c_i(f) = (\mathbf{x}_i^\top \mathbf{w} - y_i)^2$. Then we can obtain a $1 - \delta$ (say 95%) confidence interval $[\bar{X} - \epsilon, \bar{X} + \epsilon]$, where ϵ is such that $\Pr\left(\left|\bar{X} - \mathbb{E}[\bar{X}]\right| \geq \epsilon\right) \leq \delta$. If we believed the errors were Gaussian distributed with known variance σ^2, we could use a 95% Gaussian confidence interval, with $\epsilon = 1.96\sigma/\sqrt{m}$.

We liked the Gaussian interval because it required fewer samples to get a tighter interval; but sadly it is not really usable in practice. You might even be able to plot your m errors and notice they look Gaussian distributed. But, you definitely do not know their true variance. The *Student's t-distribution* is precisely designed for this setting. This distribution allows the sample variance to be used instead of the true variance. A 95% confidence interval is given by $\epsilon = t_{\delta,m-1} S_m/\sqrt{m}$ with the unbiased (Bessel-corrected) sample variance $S_m^2 = \frac{1}{m}\sum_{i=1}^{m}(c_i(f) - \bar{X})^2$. The constant $t_{\delta,m-1}$ now also depends on the number of samples, contrasting this constant for the Gaussian (which was 1.96). For $m = 2$, we have $t_{0.05,1} = 12.71$; for $m = 11$, we have $t_{0.05,10} = 2.228$; and for $m = 101$, we have $t_{0.05,100} = 1.984$. In the limit, as $m \to \infty$, this constant approach 1.96, because the distribution becomes a Gaussian distribution.

This confidence interval is useful just for evaluating the performance of one model. But, we can also use them to compare two models. If two intervals do not overlap, then we can say that they are different with high probability: that they are statistically significantly different. Assume f_1 has error $\bar{X}_1$ and f_2 has error $\bar{X}_2$, with correspondingly intervals given by ϵ_1 and ϵ_2. Then if $\bar{X}_1 + \epsilon_1 < \bar{X}_2 - \epsilon_2$, then we can say that f_1 is statistically significantly better than f_2 with confidence level δ.

8.3.2 Parametric Tests

Using confidence intervals is one of the simplest, but also least powerful statistical significance tests. We can do better by considering tests designed to compared two means. For now, let's start with a simple case, where we compare two models using the binomial test. Imagine you do not care about precise errors, but rather just want to rank the algorithms by saying which did better or worse. We can carry out such a comparison using a counting test: for each sample i, we award a win to f_1 if it has lower error and vice versa. In the case of exactly the same performance, we can provide a win/loss randomly.

	1	2	3	4		$m-1$	m
f_1	1	0	1	1	$\cdots$	0	1
f_2	0	1	0	0		1	0

Table 8.1: A counting test where models f_1 and f_2 are compared on a set of m independent samples. A model with better performance on a particular sample collects a win (1), whereas the other algorithm collects a loss (0).

Our goal is to provide statistical evidence that say model f_1 is better than model f_2. Suppose f_1 has k wins out of m and f_2 has $m-k$ wins, as shown in Table 8.1. Assume $k > m-k$, as otherwise we would be asking if f_2 is statistically significantly better than f_1. We would like to evaluate the null hypothesis H_0 that f_1 and f_2 have the same performance by providing an alternative hypothesis H_1 that f_1 is better than f_2. In short,

$$H_0\text{: quality}(f_1) = \text{quality}(f_2)$$
$$H_1\text{: quality}(f_1) > \text{quality}(f_2)$$

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 $\beta = 1/2$. Now, we can express the probability that f_1 would have collected k wins or more under the null hypothesis using the binomial distribution

$$p = \Pr(f_1 \text{ gets at least } k \text{ wins}) = \sum_{i=k}^{m} \binom{m}{i} \beta^i (1-\beta)^{m-i}$$

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. It reflects how likely it is that f_1 would have been able to get so many wins, i.e., get a least k wins.

This probability p is referred to as the p-value. A typical approach in these cases is to establish a significance value, say, $\alpha = 0.05$ and reject the null hypothesis if $p \leq \alpha$. For sufficiently low p-values, we may conclude that there is sufficient evidence that f_1 is better than f_2. The p-value represents the likelihood of observing these outcomes—observing the evidence—if the null hypothesis is true. If the p-value is very small, this says that the probability of that evidence is very small, and so it suggests you were wrong to think the null hypothesis accurately describes the world. Instead, it is more reasonable to conclude your model of the world—the null hypothesis—is wrong. If the p-value is greater than α we say that there is insufficient evidence for rejecting[1] H_0.

The choice of the significance threshold α is somewhat arbitrary. A value of 5% is typical, 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

[1] Note that this does not mean that we accept the null hypothesis. Rather, we assumed it was true and evidence did not contradict that fact. But, absence of evidence is not a proof: just because it was not disproved, does not mean that it was proved.

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*. This test can be used 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 $m-1$ 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. Or, in this setting, t would be negative, so we check 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 $p = Pr(T > |t|)$. Note that this two-tailed test will always have a bigger p-value than the one-sided tests.

	1	2	3	4		$m-1$	m
f_1	0.11	0.08	0.15	0.12	$\cdots$	0.07	0.09
f_2	0.10	0.09	0.11	0.12	$\cdots$	0.10	0.09
performance difference 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, i.e., d = performance(f_1) - performance(f_1). These differences are used for the paired t-test.

8.3.3 How to Choose the Statistical Significance Test

We gave two examples of test: the binomial test and the paired t-test. These tests make parametric assumptions. The binomial test requires that the compared values are 0, 1 values. The paired t-test assumes the difference in errors follows a Student's t-distribution, which is satisfied if the paired samples are normally distributed with equal variance. However, these conditions are not always satisfied, in which case other tests are more suitable. Further, there are some tests that do not make distributional assumptions, and rather are non-parametric. For a summary of which test to use in different settings, see [9, Section 6.3]

The choice of the test comes down to satisfying assumptions, and the power of the test. The power of the test is the ability for the test to reject the null hypothesis, if it should be rejected. The approach using non-overlapping confidence intervals is a low-power test, because it does not take into account the paired errors for the two models. When a test fails to reject the null hypothesis, when it should have been rejected, this is called a Type II error (a false negative outcome). If the test is a low-power test, then it is more likely to commit a Type II error. On the other hand, if a test is used when assumptions are violated, then we might falsely conclude that we can reject the null hypothesis, when in fact we should not have. This is called a Type I error (a false positive outcome). For example, if we make a relatively strong parametric assumption that the errors are Gaussian, then we have more power to reject the null hypothesis but might commit a Type I error if the errors are in fact not normally distributed.

These choices for statistical tests are similar to the choices we make when learning models: strong assumptions can enable faster learning, but are more biased and can lead to poorer predictions, whereas very general models can produce accurate predictions, but might need a lot of data. This choice is even more difficult for statistical significance tests, where the amount of available data is often highly limited—running experiments is expensive.

Chapter 9

Regularization and Constraining the Hypothesis Space

In this chapter, we discuss how regularization can be used to mitigate issues of overfitting. In particular, we discuss both regularizing the weights, as well as restricting the function class. We then discuss a foundational concept in machine learning: the bias-variance trade-off.

9.1 Regularization as MAP

So far, we have discussed linear regression in terms of maximum likelihood. But, as before, we can also propose a MAP objective. This means we specify a prior over $\mathbf{w}$. In particular, we 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 9.1.

Let's start with the Gaussian prior. We assume each element w_j has a Gaussian prior $\mathcal{N}(0, \sigma^2/\lambda)$, with zero covariance between the weights, for some $\lambda > 0$ and under the assumption that $p(y|\mathbf{x}) = \mathcal{N}(\mathbf{x}^\top \mathbf{w}, \sigma^2)$. The choice of the constant σ^2/λ for the prior variance is explained below. By picking a Gaussian on each w_j, we get the prior $p(\mathbf{w}) = p(w_1)p(w_2)\ldots p(w_d)$. Taking the log of this zero-mean Gaussian prior, we get

$$\begin{aligned}
-\ln p(\mathbf{w}) &= -\sum_{j=1}^{d} \ln p(w_j) = -\sum_{j=1}^{d} \ln\left(\frac{1}{\sqrt{2\pi\sigma^2/\lambda}} \exp(-\frac{w_j^2}{2\sigma^2/\lambda}\right) \\
&= -\sum_{j=1}^{d} -\tfrac{1}{2}\ln(2\pi\sigma^2/\lambda) - \frac{w_j^2}{2\sigma^2/\lambda} \\
&= \tfrac{d}{2}\ln(2\pi\sigma^2/\lambda)) + \frac{\lambda}{2\sigma^2}\sum_{j=1}^{d} w_j^2
\end{aligned}$$

We can drop the first term, which does not affect the selection of $\mathbf{w}$ since it is constant. We can combine the negative log-likelihood and the negative log prior. Then ignoring constants, we can add up the negative log-likelihood and negative log to the prior to get

$$\begin{aligned}
\underset{\mathbf{w}\in\mathbb{R}^{d+1}}{\operatorname{argmin}} -\ln(p(\mathbf{y}|\mathbf{X},\mathbf{w})) - \ln p(\mathbf{w}) &= \underset{\mathbf{w}\in\mathbb{R}^{d+1}}{\operatorname{argmin}} \frac{1}{2\sigma^2}\sum_{i=1}^{n}\left(\mathbf{x}_i^\top - y_i\right)^2 + \frac{\lambda}{2\sigma^2}\sum_{j=1}^{d} w_j^2 \\
&= \underset{\mathbf{w}\in\mathbb{R}^{d+1}}{\operatorname{argmin}} \tfrac{1}{2}\sum_{i=1}^{n}\left(\mathbf{x}_i^\top \mathbf{w} - y_i\right)^2 + \frac{\lambda}{2}\sum_{j=1}^{d} w_j^2.
\end{aligned}$$

Recall that $\mathbf{x}_i^\top \mathbf{w} = \sum_{j=0}^{d} w_j x_{ij}$, which gives the prediction $\hat{y}_i$. Notice that the regularization does not include w_0, because the intercept term only shifts the function. It does not increase the complexity of the function, and so does not notably contribute to overfitting. It is preferable to avoid regularizing w_0, so that it can accurately learn the mean value of the target across $\mathbf{x}$.

Exercise 10: Show that the learned $w_0 = \frac{1}{n}\sum_{i=1}^n y_i$. Notice that this is approximating $\mathbb{E}[Y]$. You can use this to conclude that if y_i is centered across all samples, then we did not need to add an intercept term (i.e., $w_0 = 0$). Centering involves taking the average values across samples, and subtracting it from each point: $\tilde{y}_i = y_i - \frac{1}{n}\sum_{i=1}^n y_i$. □

In summary, if we assume that each weight, except w_0, has a zero-mean Gaussian prior $\mathcal{N}(0, \lambda^{-1}\sigma^2)$, then we get the following ℓ_2-regularized problem[1], also called ridge regression:

$$c(\mathbf{w}) = \tfrac{1}{2}\sum_{i=1}^n \left(\mathbf{x}_i^\top - y_i\right)^2 + \frac{\lambda}{2}\sum_{j=1}^d w_j^2 \tag{9.1}$$

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. Correspondingly, larger λ corresponds to a smaller covariance in the prior, pushing the weights to stay near zero. The MAP estimate, therefore, has to balance between this prior on the weights, and fitting the observed data.

Similarly to linear regression, we can take the gradient of this objective to get a system of $d+1$ equations. We can obtain a closed form solution, but will typically use stochastic gradient descent. Instead of using cumulative errors, we will again use an average error for the first term to get the more commonly used objective for ridge regression:

$$c(\mathbf{w}) = \frac{1}{2n}\sum_{i=1}^n \left(\mathbf{x}_i^\top - y_i\right)^2 + \frac{\lambda}{2}\sum_{j=1}^d w_j^2 \tag{9.2}$$

Notice that this objective is actually different from the one above, in the sense that the λ has a different scale. For a fixed λ, as the number of samples increases in Equation (9.1), the regularizer plays a diminishing role. This is the typical for MAP, where prior information is gradually washed out by more and more data. In Equation (9.2), however, even with more data, we always include the same amount of regularization. In practice, if you know you have lots of data, you will likely set λ to be small and so effectively the objectives in (9.1) and (9.2) would not be too different.

The form in Equation (9.2) is more amenable for our stochastic gradient descent solution approach, which is why we pick that instead of (9.1). We can write this objective as an average of $c_1, c_2, \ldots, c_n$ using $c_i(\mathbf{w}) = \frac{1}{2}\left(\mathbf{x}_i^\top - y_i\right)^2 + \frac{\lambda}{2}\sum_{j=1}^d w_j^2$ because

$$\begin{aligned}
\frac{1}{n}\sum_{i=1}^n c_i(\mathbf{w}) &= \frac{1}{n}\sum_{i=1}^n \left[\tfrac{1}{2}\left(\mathbf{x}_i^\top - y_i\right)^2 + \frac{\lambda}{2}\sum_{j=1}^d w_j^2\right] \\
&= \frac{1}{2n}\sum_{i=1}^n \left(\mathbf{x}_i^\top - y_i\right)^2 + \frac{1}{n}\sum_{i=1}^n \frac{\lambda}{2}\sum_{j=1}^d w_j^2 \\
&= \frac{1}{2n}\sum_{i=1}^n \left(\mathbf{x}_i^\top - y_i\right)^2 + \frac{\lambda}{2}\sum_{j=1}^d w_j^2 = c(\mathbf{w})
\end{aligned}$$

[1] It is called ℓ_2-regularized linear regression, because the regularizer uses an ℓ_2-norm on the weights. See the notation at the beginning of these notes, for the definitions of norms on vectors.

The gradient for each term c_i is composed of the following partial derivatives

$$\frac{\partial c_i(\mathbf{w})}{\partial w_0} = \left(\mathbf{x}_i^\top - y_i\right)$$

and for $j \in \{1, 2, \ldots, d\}$

$$\frac{\partial c_i(\mathbf{w})}{\partial w_j} = \left(\mathbf{x}_i^\top - y_i\right) x_{ij} + \lambda w_j$$

because

$$\frac{\partial \frac{\lambda}{2} \sum_{k=1}^d w_k^2}{\partial w_j} = \frac{\lambda}{2} \sum_{k=1}^d \frac{\partial w_k^2}{\partial w_j} = \frac{\lambda}{2} \frac{\partial w_j^2}{\partial w_j} = \lambda w_j.$$

Each stochastic gradient descent update is

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta_t \mathbf{g}_t$$

where $\mathbf{g}_t = \nabla c_i(\mathbf{w})$ for a random sample i, with

$$\nabla c_i(\mathbf{w}) = \begin{bmatrix} (\mathbf{x}_i^\top - y_i) \\ (\mathbf{x}_i^\top - y_i)\, x_{i1} + \lambda w_1 \\ (\mathbf{x}_i^\top - y_i)\, x_{i2} + \lambda w_2 \\ \vdots \\ (\mathbf{x}_i^\top - y_i)\, x_{id} + \lambda w_d \end{bmatrix}$$

Exercise 11: Write down the mini-batch gradient descent update. □

We can go through the same procedure with a different prior: a Laplace prior. If we go through similar steps as above, we get an ℓ_1 penalized objective

$$c(\mathbf{w}) = \tfrac{1}{n} \sum_{i=1}^n \left(\mathbf{x}_i^\top - y_i\right)^2 + \lambda \sum_{j=1}^d |w_j| \tag{9.3}$$

which is often called the Lasso. We put a Laplace prior on each weight $p(w_j) = \frac{1}{2b} \exp(-\frac{|w_j - \mu|}{b})$ with parameters $\mu = 0$ and scale $b = \sigma^2/\lambda$. This results in putting an ℓ_1 regularizer on the weights, which sums up the absolute values of the weights.

Exercise 12: Derive Equation (9.3) using the MAP formulation with the given Laplace prior, similarly to how it was done for MAP with a Gaussian prior on the weights. □

As with the ℓ_2 regularizer for ridge regression, the ℓ_1 regularizer penalizes large values in $\mathbf{w}$. However, it also produces more sparse solutions, where entries in $\mathbf{w}$ are zero. This preference can be seen in Figure 9.1, where the Laplace distribution is more concentrated around zero. In practice, however, this preference is even stronger than implied by the distribution, due to how the spherical least-squares loss and the ℓ_1 regularizer interact.

Forcing entries in $\mathbf{w}$ to zero has the effect of feature selection, because zeroing entries in $\mathbf{w}$ is equivalent to removing the corresponding feature. Consider the dot product

$$\mathbf{x}^\top \mathbf{w} = \sum_{j=0}^d x_j w_j = \sum_{j: w_j \neq 0} x_j w_j.$$

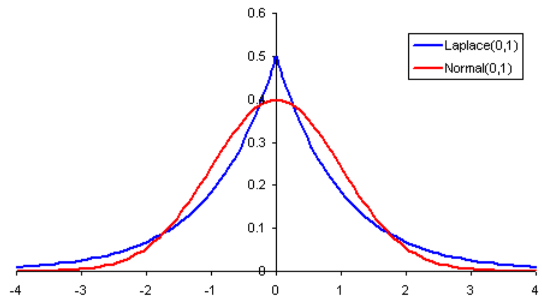


Figure 9.1: A comparison between Gaussian and Laplace priors. Both prefers values to be near zero, but the Laplace prior more strongly prefers the values to equal zero.

This is equivalent to simply dropping entries in $\mathbf{x}$ and $\mathbf{w}$ where $w_j = 0$.

For the Lasso, we no longer have a closed-form solution. We do not have a closed form solution, because we cannot solve for $\mathbf{w}$ in closed-form that provides a stationary point. Instead, we use gradient descent to compute a solution to $\mathbf{w}$. The ℓ_1 regularizer, however, is non-differentiable at 0. Understanding how to optimize this objective requires a bit more optimization background; we leave it for a future course.

9.2 Expectation and variance for the regression solutions

A natural question to ask is how this regularization parameter can be selected, and the impact on the final solution vector. The selection of this regularization parameter leads to a bias-variance trade-off. To understand this trade-off, we need to understand what it means for the solution to be biased, and how to characterize the variance of the solution, across possible datasets.

Let us begin with understanding the bias and variance of the non-regularized solution. For simplicity in the derivation, let's look only at the univariate setting: input $x \in \mathbb{R}$ and weights $w \in \mathbb{R}$, with $f(x) = xw$. For this analysis, we start by presuming the distributional assumptions behind linear regression are true. This means that there exists a true parameter ω such that for each of the data points $Y_i = \omega X_i + \varepsilon_i$, where the ε_j are i.i.d. random variables drawn according to $\mathcal{N}(0, \sigma^2)$. We can characterize the MLE weights (estimator) w_{MLE} as a random variable, where the randomness is across possible datasets that could have been observed. In this sense, we are considering the dataset $\mathcal{D}$ to be a random variable, and the solution $w_{\text{MLE}}(\mathcal{D})$ from that dataset as a function of this random variable.

We can show that $w_{\text{MLE}}(\mathcal{D})$ is an unbiased estimator of ω. To do so, we will need the closed form solution

$$w_{\text{MLE}}(\mathcal{D}) = \frac{\sum_{i=1}^n X_i Y_i}{\sum_{i=1}^n X_i^2} \tag{9.4}$$

For simplicity of notation, we will use $S_n \overset{\text{def}}{=} \sum_{i=1}^n X_i^2$. Then we have that

$$
\begin{aligned}
\mathbb{E}[w_{\text{MLE}}(\mathcal{D})] &= \mathbb{E}\left[\frac{\sum_{i=1}^n X_i Y_i}{S_n}\right] \\
&= \mathbb{E}\left[\frac{\sum_{i=1}^n X_i(\omega X_i + \varepsilon_i)}{S_n}\right] && \triangleright \text{ because } Y_i = \omega X_i + \varepsilon_i \\
&= \mathbb{E}\left[\frac{\sum_{i=1}^n (\omega X_i^2 + X_i \varepsilon_i)}{S_n}\right] \\
&= \mathbb{E}\left[\frac{\omega \sum_{i=1}^n X_i^2 + \sum_{i=1}^n X_i \varepsilon_i}{S_n}\right] \\
&= \mathbb{E}\left[\frac{\omega S_n}{S_n}\right] + \mathbb{E}\left[\frac{\sum_{i=1}^n X_i \varepsilon_i}{S_n}\right] && \triangleright \text{ by linearity of expectation} \\
&= \mathbb{E}[\omega] + \sum_{i=1}^n \mathbb{E}\left[\varepsilon_i \frac{X_i}{S_n}\right] \\
&= \omega + \sum_{i=1}^n \mathbb{E}[\varepsilon_i]\mathbb{E}\left[\frac{X_i}{S_n}\right] && \triangleright\ \omega \text{ not random and } \varepsilon_i \text{ independent of all } X_i \\
&= \omega && \triangleright \text{ because } \mathbb{E}[\varepsilon_i] = 0
\end{aligned}
$$

Therefore, we can conclude that $\mathbb{E}[w_{\text{MLE}}(\mathcal{D})] = \omega$ and so $w_{\text{MLE}}(\mathcal{D})$ is an unbiased estimator.

We can similarly characterize the variance, and obtain

$$
\begin{aligned}
\text{Var}[w_{\text{MLE}}(\mathcal{D})] &= \mathbb{E}\left[(w_{\text{MLE}}(\mathcal{D}) - \omega)^2\right] \\
&= \mathbb{E}\left[w_{\text{MLE}}(\mathcal{D})^2\right] - \omega^2
\end{aligned}
$$

Above we showed that $w_{\text{MLE}}(\mathcal{D}) = \omega + \sum_{i=1}^n \varepsilon_i \frac{X_i}{S_n}$. Again, for simplicity of notation, define this residual term $R_n \overset{\text{def}}{=} \sum_{i=1}^n \varepsilon_i \frac{X_i}{S_n}$. Then we get

$$
\begin{aligned}
w_{\text{MLE}}(\mathcal{D})^2 &= (\omega + R_n)^2 \\
&= \omega^2 + 2\omega R_n + R_n^2
\end{aligned}
$$

We can further show that

$$
\mathbb{E}[\omega R_n] = \omega \mathbb{E}[R_n] = \omega \sum_{i=1}^n \mathbb{E}[\varepsilon_i]\mathbb{E}\left[\frac{X_i}{S_n}\right] = 0
$$

as we showed above when characterizing the expectation of $w_{\text{MLE}}(\mathcal{D})$. We can use the law of total probability to show that

$$
\mathbb{E}[R_n^2] = \sigma^2 \mathbb{E}[S_n^{-1}]
$$

We leave this as an exercise. Putting this all together, we get that

$$
\begin{aligned}
\text{Var}[w_{\text{MLE}}(\mathcal{D})] &= \mathbb{E}\left[w_{\text{MLE}}(\mathcal{D})^2\right] - \omega^2 \\
&= \omega^2 + 0 + \mathbb{E}[R_n^2] - \omega^2 \\
&= \sigma^2 \mathbb{E}[S_n^{-1}] \\
&= \sigma^2 \mathbb{E}[\frac{1}{n} C_n^{-1}] && \triangleright \text{ for } C_n \overset{\text{def}}{=} \frac{1}{n}\sum_{i=1}^n X_i^2
\end{aligned}
$$

The last format is given in terms of the sample average estimate C_n, which is essentially a sample average estimate of the variance for X_i. (It would be a variance estimate, if it was centered around the mean.) This term reflects the variability in X. For a small number of samples, C_n could vary widely, and could be very small. The inverse in the above can be very big, and so the variance for $w_{\text{MLE}}(\mathcal{D})$ can be big for a small amount of data. This implies that, across datasets, the solution $w_{\text{MLE}}(\mathcal{D})$ can vary widely. This behavior is not desirable: if our solution could be very different across several different random subsets of data, we cannot be confident in any one of these solutions. Notice that as n get bigger, the variance decreases proportionally to n^{-1}, because of the $\frac{1}{n}$ in front of C_n.

The regularized solution, on the other hand, is much less likely to have high covariance, but will no longer be unbiased. Let $w_{\text{MAP}}(\mathcal{D})$ be the MAP estimate for the ℓ_2 regularized problem with some $\lambda > 0$. As above, we can write the MAP estimate as a closed form solution

$$w_{\text{MAP}}(\mathcal{D}) = \frac{\sum_{i=1}^n X_i Y_i}{\lambda + S_n} \tag{9.5}$$

Then, using similar steps to above we get

$$\begin{aligned}
\mathbb{E}[w_{\text{MAP}}(\mathcal{D})] &= \mathbb{E}\left[\frac{\sum_{i=1}^n X_i Y_i}{\lambda + S_n}\right] \\
&= \mathbb{E}\left[\frac{\omega S_n}{\lambda + S_n}\right] + \mathbb{E}\left[\frac{\sum_{i=1}^n X_i \varepsilon_i}{\lambda + S_n}\right] \\
&= \omega \mathbb{E}\left[\frac{S_n}{\lambda + S_n}\right] + 0 \\
&\neq \omega
\end{aligned}$$

when $\lambda > 0$. Notice that if $\lambda = 0$, then $w_{\text{MAP}}(\mathcal{D})$ is unbiased. In fact, it simply correspond to the MLE solution for $\lambda = 0$, so it makes sense that it is unbiased for $\lambda = 0$. The bias is determined by how far $\mathbb{E}\left[\frac{S_n}{\lambda + S_n}\right]$ is from 1. As $\lambda \to 0$, the solution becomes less and less biased. As $\lambda \to \infty$, the solution becomes maximally biased with $\mathbb{E}\left[\frac{S_n}{\lambda + S_n}\right] \to 0$.

We can also characterize the variance of $w_{\text{MAP}}(\mathcal{D})$. We leave the steps as an exercise. Again, for simplicity of notation, let's define $C_{n,\lambda} = \frac{1}{n}(\lambda + S_n)$. Then variance is

$$\text{Var}[w_{\text{MAP}}(\mathcal{D})] = \sigma^2 \mathbb{E}\left[\tfrac{1}{n} C_{n,\lambda}^{-1} C_n C_{n,\lambda}^{-1}\right]$$

Notice now that even if C_n is very small, it does not cause the variance to become very big because we are not inverting it. Instead, we use the inverse of $C_{n,\lambda}$. This inverse is always smaller than $1/\lambda$, because we increase the denominator by λ. Therefore, for reasonably large λ, the variance will not be very big and it should be notably smaller than $w_{\text{MLE}}(\mathcal{D})$.

The reason we care about the bias and variance is that the expected mean-squared error to the true weights can be decomposed into the bias and variance. We saw this in Section 3.5, when we talked about sample average estimators. As depicted in Figure 9.2, there is an optimal choice of λ that minimizes this bias-variance trade-off—if we could find it. We can show the same decomposition for the weights for regression

$$\mathbb{E}\left[\|\mathbf{w}(\mathcal{D}) - \boldsymbol{\omega}\|_2^2\right] = \mathbb{E}\left[\sum_{j=1}^{d}(w_j(\mathcal{D}) - \omega_j)^2\right]$$
$$= \sum_{j=1}^{d}\mathbb{E}\left[(w_j(\mathcal{D}) - \omega_j)^2\right]$$

where we can then further simplify this inner term

$$\mathbb{E}\left[(w_j(\mathcal{D}) - \omega_j)^2\right] = \mathbb{E}\left[(w_j(\mathcal{D}) - \mathbb{E}\left[w_j(\mathcal{D})\right] + \mathbb{E}\left[w_j(\mathcal{D})\right] - \omega_j)^2\right]$$
$$= \mathbb{E}\left[(w_j(\mathcal{D}) - \mathbb{E}\left[w_j(\mathcal{D})\right])^2\right] + \mathbb{E}\left[(\mathbb{E}\left[w_j(\mathcal{D})\right] - \omega_j)^2\right]$$

where the second step follows from the fact that

$$-2\mathbb{E}\left[(w_j(\mathcal{D}) - \mathbb{E}\left[w_j(\mathcal{D})\right])(\mathbb{E}\left[w_j(\mathcal{D})\right] - \omega_j)\right] = (\mathbb{E}\left[w_j(\mathcal{D})\right] - \omega_j)\mathbb{E}\left[w_j(\mathcal{D}) - \mathbb{E}\left[w_j(\mathcal{D})\right]\right]$$
$$= 0.$$

The first term above in $\mathbb{E}\left[(w_j(\mathcal{D}) - \omega_j)^2\right]$ is the variance of the jth weight and the second term is the bias of the jth weight, where $\mathbb{E}\left[(\mathbb{E}\left[w_j(\mathcal{D})\right] - \omega_j)^2\right] = (\mathbb{E}\left[w_j(\mathcal{D})\right] - \omega_j)^2$ because nothing is random in this term so the outer expectation is dropped. This gives

$$\mathbb{E}\left[\|\mathbf{w}(\mathcal{D}) - \boldsymbol{\omega}\|_2^2\right] = \sum_{j=1}^{d}\mathbb{E}\left[(w_j(\mathcal{D}) - \omega_j)^2\right]$$
$$= \sum_{j=1}^{d}(\mathbb{E}\left[w_j(\mathcal{D})\right] - \omega_j)^2 + \mathrm{Var}\left[w_j(\mathcal{D})\right]$$

showing that the expected mean-squared error to the true weight vector $\boldsymbol{\omega}$ decomposes into the squared bias $\mathbb{E}\left[w_j(\mathcal{D})\right] - \omega_j$ and the variance $\mathrm{Var}\left[w_j(\mathcal{D})\right]$. The bias-variance trade-off reflects the fact that we could potentially reduce the mean-squared error by incurring some bias, as long as the variance is decreased more than the squared bias.

Remark: We do not directly optimize the bias-variance trade-off. We cannot actually measure the bias, so we do not directly minimize these terms. Rather, this decomposition guides how we select models.

9.3 The Bias-Variance Trade-off

Above we assumed that the true model was linear, and so the only bias introduced was from the regularization. This assumed that the hypothesis space of linear functions included the true function, and that the bias introduced was only due to regularization. In reality, when using linear regression with regularization, we are introducing bias both from selecting a simpler function class and from the regularization. If the true function is not linear, then we cannot compare the learned weights for a linear function directly to the true function. If a powerful basis is used to first transform the data, then we can learn nonlinear functions even though the solution uses linear regression. In this case, it is feasible that this function class is sufficiently powerful and includes the true function, and that the bias is mostly due

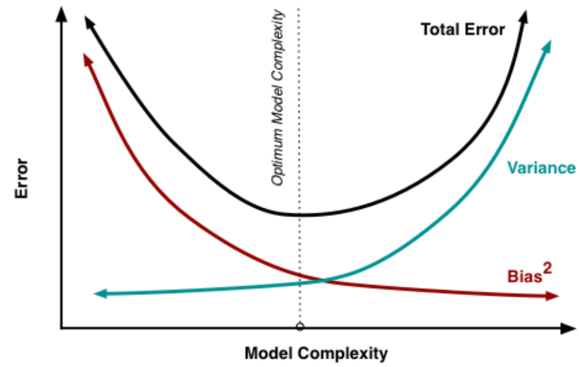


Figure 9.2: The bias-variance trade-off. Image obtained from: http://scott.fortmann-roe.com/docs/BiasVariance.html

to regularization. But, in general, it will be difficult to guarantee that we have specified a function class that includes the true function, and it will be difficult to directly compare our parameters to true parameters (which may not even be of the same dimension).

We can more generally talk about bias and variance by considering instead the reducible error. In fact, the bias-variance trade-off is all about reducing the reducible error. (Remember, we cannot reduce the irreducible error—the name says it all—by improving how we estimate the function.) We can define a more general bias-variance decomposition that compares function outputs rather than parameter vectors. Recall the reducible error corresponds to $\mathbb{E}\left[(f_{\mathcal{D}}(\boldsymbol{X}) - f(\boldsymbol{X}))^2\right]$, where $f(\boldsymbol{X})$ is the optimal function, i.e., $f(\mathbf{x}) = \mathbb{E}[Y|\mathbf{x}]$ for the squared cost. We previously discussed this reducible error for a fixed function, with expectation only over $\boldsymbol{X}$. But now we additionally consider the fact that $f_{\mathcal{D}}$ is random, and we can reason about its expectation and variance for a given $\mathbf{x}$.

Let's start by only considering the expected mean-squared error, for a given input $\mathbf{x}$. Using similar steps to the decomposition above, we get

$$\mathbb{E}\left[(f_{\mathcal{D}}(\mathbf{x}) - f(\mathbf{x}))^2)\right] = (\mathbb{E}\left[f_{\mathcal{D}}(\mathbf{x})\right] - f(\mathbf{x}))^2 + \mathrm{Var}\left[f_{\mathcal{D}}(\mathbf{x})\right].$$

Notice that in the second line, the expectation is now inside the squared distance; this term corresponds to the squared bias. The bias here reflects the output of the estimated function $f_{\mathcal{D}}(\mathbf{x})$, in expectation across all datasets $\mathcal{D}$. The variance term reflects how much the prediction for $\mathbf{x}$ can vary, if we learn on different iid datasets. This decomposition of the mean-squared error into a squared bias and variance is not obvious, but does follow similar steps to above. It is left as an exercise.

The above generalization highlights that one of the ways we balance bias and variance is actually in the selection of the function class. If we select a simple function class, the class is likely not large enough—not powerful enough—to represent the true function. This introduces some bias, but likely also has lower variance, because that simpler function class is less likely to overfit to any one dataset. If this class is too simple, then we might be suffering from underfitting. On the other hand, if we select a more powerful function class, that does contain the true function, we may not have any bias but could have high variance due to the ability to find a function in your large class that overfits a given dataset. Though we have the ability to learn a highly accurate function, it will be difficult to actually find that function amongst this larger class. Instead, one is likely to select a model that overfits to the given data, and does not generalize to new data (i.e., performs poorly on new data).

Finding the balance between bias and variance, and between underfitting and overfitting, is a core problem in machine learning. Our goal is to identify the true function, and in some cases the data may be insufficient for identification. For example, imagine you are given a dataset of images, where the color red has no impact on prediction accuracy. Your classifier, though, does not know that this property is irrelevant and may use it to better fit the data. If there were multiple instances of the same picture, with and without the color red, it might be able to learn that that property is not relevant. But that is too much to hope for. Instead, we build-in some prior knowledge into the types of functions we learn to acknowledge that the given data is unlikely to be sufficient to perfectly identify the model. That prior knowledge need not be specific to the problem; it could be as simple as preferring to use a minimal set of features in the observed data. Understanding what this prior knowledge should be—understanding inductive biases—remains an important question.

Chapter 10

Logistic Regression and Linear Classifiers

In Chapter 6, when introducing prediction, we presented a classifier as a function $f : \mathcal{X} \to \mathcal{Y}$ and showed that a reasonable goal to obtain a good classifier is to approximate $p(y|\mathbf{x})$. Similarly to linear regression, we need to figure out how to parameterize $p(y|\mathbf{x})$. We know $p(y|\mathbf{x})$ must be a (conditional) Bernoulli distribution, because Y is a binary variable. The parameter for a Bernoulli distribution is $\alpha(\mathbf{x}) = p(y = 1|\mathbf{x})$, the success probability.

One of the simplest approaches to learning this distribution is given by *logistic regression*. The idea is to parameterize $p(y = 1|\mathbf{x})$ using a sigmoid function on $\mathbf{x}^\top\mathbf{w}$, i.e., $(1+e^{-\mathbf{x}^\top\mathbf{w}})^{-1}$, shown in Figure 10.1. In this chapter, we explain linear classifiers, why logistic regression produces a linear classifier and how to estimate the parameters $\mathbf{w}$ for logistic regression.

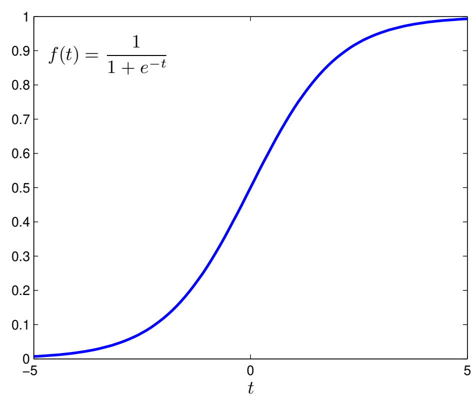


Figure 10.1: Sigmoid function in the interval $[-5, 5]$.

10.1 Linear Classifiers

Suppose we are interested in building a linear classifier $f : \mathbb{R}^d \to \{0, +1\}$. 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. An example of a classifier with a linear decision surface is shown in Figure 10.2. The two half-spaces act as decision regions for the positive and negative examples, respectively. For a given $\mathbf{x}$, if $\mathbf{x}^\top\mathbf{w} > 0$, then $\mathbf{x}$ is classified as a positive. If $\mathbf{x}^\top\mathbf{w} < 0$, then $\mathbf{x}$ is classified as a negative.

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

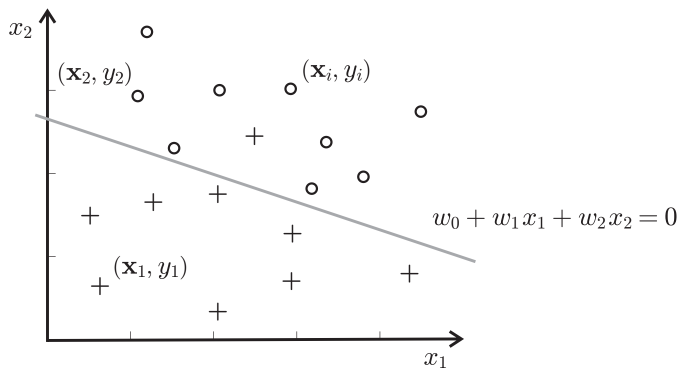


Figure 10.2: A data set in $\mathbb{R}^2$ consisting of nine positive and nine negative examples. The gray line represents a linear decision surface in $\mathbb{R}^2$. The decision surface does not perfectly separate positives from negatives.

fraction of examples on the incorrect side of the decision surface. Alternatively, the goal of the training algorithm may be to directly estimate the conditional distribution $p(y|\mathbf{x})$, such as is done by logistic regression.

As in regression, we add a component $x_0 = 1$ to each input $(x_1, \ldots, x_d)$ to model the intercept term. Notice that, without an intercept term, the linear classifier would be required to go through the origin, significantly skewing the solution. In Figure 10.2, for example, if $w_0 = 0$, then $w_1x_1 + w_2x_2 = 0$ for $(x_1 = 0, x_2 = 0)$. However, the line depicted clearly should not go through the origin.

10.2 What Logistic Regression Learns

Let us consider binary classification in $\mathbb{R}^d$, where $\mathcal{X} = \mathbb{R}^{d+1}$ and $\mathcal{Y} = \{0, 1\}$. The Bernoulli distribution over Y, with α a function of $\mathbf{x}$, is

$$p(y|\mathbf{x}) = \begin{cases} \left(\frac{1}{1+e^{-\boldsymbol{\omega}^\top \mathbf{x}}}\right) & \text{for } y = 1 \\ \left(1 - \frac{1}{1+e^{-\boldsymbol{\omega}^\top \mathbf{x}}}\right) & \text{for } y = 0 \end{cases} \tag{10.1}$$
$$= \sigma(\mathbf{x}^\top \mathbf{w})^y (1 - \sigma(\mathbf{x}^\top \mathbf{w}))^{1-y}$$

where $\boldsymbol{\omega} = (\omega_0, \omega_1, \ldots, \omega_d)$ is a set of unknown coefficients we want to recover (or learn). Notice that our prediction is $\sigma(\boldsymbol{\omega}^\top \mathbf{x})$, and that it satisfies

$$p(y = 1|\mathbf{x}) = \sigma(\boldsymbol{\omega}^\top \mathbf{x}).$$

Therefore, as with many binary classification approaches, our goal is to predict the probability that the class is 1; given this probability, we can infer $p(y = 0|\mathbf{x}) = 1 - p(y = 1|\mathbf{x})$.

The function learned by logistic regression returns a probability, rather than an explicit prediction of 0 or 1. Therefore, we have to take this probability estimate and convert it to a suitable prediction of the class. For a previously unseen data point $\mathbf{x}$ and a set of learned coefficients $\mathbf{w}$, we simply calculate the conditional probability as

$$p(y = 1|\mathbf{x}, \mathbf{w}) = \frac{1}{1 + e^{-\mathbf{x}^\top \mathbf{w}}}.$$

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 ($\hat{y} = 0$). The predictor maps a $(d+1)$-dimensional vector $\mathbf{x} = (x_0 = 1, x_1, \ldots, x_d)$ into a zero or one. Notice that the logistic regression classifier is a linear classifier, despite the fact that the sigmoid is non-linear. This is because $p(y = 1|\mathbf{x}, \mathbf{w}) \geq 0.5$ only when $\mathbf{x}^\top \mathbf{w} \geq 0$. The expression $\mathbf{x}^\top \mathbf{w} = 0$ represents the equation of a hyperplane that separates positive and negative examples.

Notice that, even if logistic regression can perfectly model $p(y = 1|\mathbf{x})$, this does not mean we obtain perfect classification accuracy. Imagine you were given the true $p(y = 1|\mathbf{x})$ that generates the data. Imagine for one observation vector, $p(y = 1|\mathbf{x}) = 0.5$. This means that, for this given observation, 50% of the time is labeled positive and 50% it is labeled negative. This goes back to partial observability and irreducible error. The given observations are insufficient to perfectly characterize the outcome. Potentially, if we had obtain a richer observation vector $\mathbf{x}$ with more information, the target y might become more certain and the distribution over y more concentrated at one value. But, we are stuck with the data we have been given, and so have to recognize that sometimes a class label is simply ambiguous, even under the optimal model.

This does mean, however, that the probability values themselves can be reflective. If the probability estimates are accurate, then they provide a measure of confidence in the classification. You might be more comfortable making a health decision if the classifier $p(y = 1|\mathbf{x}) = 0.99$ rather than if $p(y = 1|\mathbf{x}) = 0.6$. Additionally, recognizing that the probabilities themselves matter, rather than just the resulting classification, can help you pick between classifiers. For example, if you have two classifiers that produce good accuracies, it is preferable to have a classifier that consistently produces probabilities near 0.9 and 0.1, rather than probabilities that hover around 0.5. This reason for this is that small perturbations are expected to have more impact on the second classifier, which could suddenly erroneously swap the labeling on an instance.

Remark: As we discuss in Chapter 8, the threshold for classification need not be 0.5. In some cases, one might care more about failing to identify a positive (e.g., failing to identify a disease); in such a case, it may be safer to err on the side of a smaller threshold, so that more instances are labeled as positive. For now, we will assume this simpler thresholding, but remain cognizant that the choice can be an important one.

10.3 Maximum Likelihood for Logistic Regression

To learn the parameters for logistic regression, we need to define an objective. We will once again use maximum likelihood to help us derive a reasonable objective. As before, 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 $p(\mathbf{x}, y) = p(y|\mathbf{x})p(\mathbf{x})$. The data is generated by randomly drawing a point $\mathbf{x}$ according to $p(\mathbf{x})$ and then sets its class label Y according to the Bernoulli distribution in (10.1). Our objective is the negative log-likelihood for the conditional distribution, scaled by the number of samples

$$c_i(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} - \ln p(y_i|\mathbf{x})$$

which we can write as $c(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n} c_i(\mathbf{w})$ where

$$\begin{aligned}
c_i(\mathbf{w}) &= -\ln p(y_i|\mathbf{x}) \qquad\qquad \triangleright\ p(y_i|\mathbf{x}) = \sigma(\mathbf{x}^\top \mathbf{w})^y (1-\sigma(\mathbf{x}^\top \mathbf{w}))^{1-y} \\
&= -\ln \sigma(\mathbf{x}^\top \mathbf{w})^y - \ln(1-\sigma(\mathbf{x}^\top \mathbf{w}))^{1-y} \\
&= -y_i \ln \sigma(\mathbf{x}_i^\top \mathbf{w}) - (1-y_i)\ln\left(1-\sigma(\mathbf{x}_i^\top \mathbf{w})\right) \\
&= \left(y_i \ln\left(\frac{1}{1+e^{-\mathbf{x}_i^\top \mathbf{w}}}\right) + (1-y_i)\ln\left(1-\frac{1}{1+e^{-\mathbf{x}_i^\top \mathbf{w}}}\right)\right).
\end{aligned}$$

This objective is typically referred to as the *cross-entropy*.

From here, you could take the derivative of each component in this sum, using the chain rule for the sigmoid. For the first component, with $p_i = \sigma(\theta_i)$,

$$\begin{aligned}
\frac{\partial y_i \ln \sigma(\mathbf{x}_i^\top \mathbf{w})}{\partial w_j} &= y_i \frac{\partial \ln \sigma(\theta_i)}{\partial \theta_i}\frac{\partial \theta_i}{w_j} \\
&= y_i \frac{\partial \ln p_i}{\partial p_i}\frac{\partial p_i}{\partial \theta_i}\frac{\partial \theta_i}{w_j} \\
&= y_i \frac{1}{p_i}\frac{\partial p_i}{\partial \theta_i}\frac{\partial \theta_i}{w_j} \\
&= y_i \frac{1}{p_i}\sigma(\theta_i)(1-\sigma(\theta_i))x_{ij} \\
&= y_i(1-\sigma(\theta_i))x_{ij}
\end{aligned}$$

because

$$\frac{\partial \sigma(\theta_i)}{\partial \theta_i} = \sigma(\theta_i)(1-\sigma(\theta_i)).$$

You can verify this step for yourself, but explicitly plugging in the definition of σ. For the second component, following similar steps, we get

$$\frac{\partial (1-y_i)\ln(1-\sigma(\mathbf{x}_i^\top \mathbf{w}))}{\partial w_j} = (y_i - 1)\sigma(\theta_i)x_{ij}$$

Summing these together and taking the negative, we end up with the gradient $(p_i - y_i)x_{ij}$.

Exercise 13: We could have slightly rearranged the objective before taking the gradient. This would lead to another path to derive the update rule for logistic regression. You can notice first that

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

giving

$$\begin{aligned}
c_i(\mathbf{w}) &= -y_i \cdot \ln\left(1+e^{-\mathbf{x}_i^\top \mathbf{w}}\right) + (1-y_i)\cdot \ln\left(e^{-\mathbf{x}_i^\top \mathbf{w}}\right) - (1-y_i)\cdot \ln\left(1+e^{-\mathbf{x}_i^\top \mathbf{w}}\right) \\
&= (y_i - 1)\,\mathbf{x}_i^\top \mathbf{w} + \ln\left(\frac{1}{1+e^{-\mathbf{x}_i^\top \mathbf{w}}}\right).
\end{aligned}$$

Derive the gradient of c starting from here. □

Unlike linear regression, there is no closed-form solution to $\nabla c(\mathbf{w}) = \mathbf{0}$. Thus, we have to proceed with iterative optimization methods, like gradient descent. We initialize $\mathbf{w}_0$ usually to a random vector (or potentially with the linear regression solution which provides a much better initial point). Because the objective is convex, the initialization only affects the number of steps, but should not prevent the gradient descent from converging to a global minimum. The stochastic gradient descent update is

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta_t \left(\sigma(\mathbf{x}_i^\top \mathbf{w}_t) - y_i\right) \mathbf{x}_i$$

and the mini-batch gradient descent update, for mini-batch $(\mathbf{x}_k, y_k), \ldots, (\mathbf{x}_{k+b}, y_{k+b})$ is

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \frac{\eta_t}{b} \sum_{i=k}^{k+b} \left(\sigma(\mathbf{x}_i^\top \mathbf{w}_t) - y_i\right) \mathbf{x}_i.$$

10.4 Issues with Minimizing the Squared Error

A natural question is why we went down this route for linear classification. Instead of explicitly assuming $p(y = 1|\mathbf{x})$ is a Bernoulli distribution and computing the maximum likelihood solution for $\sigma(\mathbf{x}^\top \mathbf{w}) = p(y = 1|\mathbf{x}, \mathbf{w})$, 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 favourite loss (the squared loss).

$$\min_{\mathbf{w}} \frac{1}{n} \sum_{i=1}^{n} \left(\sigma(\mathbf{x}_i^\top \mathbf{w}) - y_i\right)^2$$

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].

Minimization of this non-convex function, therefore, is more problematic than the convex cross-entropy. Gradient descent on the cross-entropy, with stepsizes gradually decayed, will converge to a global minimum. For this non-convex squared error between the sigmoid prediction and the true label, it will generally be impossible to ensure we can converge to the global minimum. We could try to develop some tricks, like randomly restarting the optimization a different points to find different local minima, in the hopes that one will be the global minimum. But, such a search is not very effective. This example provides some motivation for why we care about selecting our objectives in an intelligent way.

Chapter 11

Bayesian Linear Regression

Bayesian estimation involves maintaining the entire posterior distribution, $p(\mathbf{w}|\mathcal{D})$. So far, we only looked at Bayesian estimation for a marginal distribution, such as $p(x)$ a Poisson distribution with unknown parameter w corresponding to λ for the Poisson. We have only discussed how MLE and MAP extends to conditional distributions, $p(y|\mathbf{x})$. In this chapter, we make the next step: discussing Bayesian estimation for conditional distributions.

In fact, once we have looked at MAP, the extension to Bayesian estimation is not a big leap. For MAP, we already had to specify a prior to obtain $\text{argmax}_{\mathbf{w}\in\mathcal{F}}\, p(\mathbf{w}|\mathcal{D})$. For Bayesian estimation, we need to maintain the entire posterior $p(\mathbf{w}|\mathcal{D})$, not just the mode. Just as before, we simplify the explanation by only considering the univariate case: $w \in \mathbb{R}$.

Assume that $p(y|x) = \mathcal{N}(\mu = xw, \sigma^2)$ for some fixed $\sigma \in \mathbb{R}$. This is the assumption we made for linear regression, and then for MAP will a Gaussian prior on the weights. Again, let's assume a Gaussian prior on the weights $p(w) = \mathcal{N}(0, \sigma^2/\lambda)$ for some (regularization) parameter $\lambda > 0$. Then we get

$$
\begin{aligned}
p(w|\mathcal{D}) &= \frac{p(\mathcal{D}|w)p(w)}{p(\mathcal{D})} \\
&= \frac{p(w)\prod_{i=1}^{n} p(y_i|x_i, w)}{\int p(w)\prod_{i=1}^{n} p(y_i|x_i, w)dw}
\end{aligned}
$$

As in Section 5.2, computing the posterior is complicated by the integral in the denominator. In some cases, though, this integral can be solved analytically, and the posterior has a simple known form. This was the case with *conjugate priors*. For a given $p(y|x, w)$, a conjugate prior $p(w)$ is one where the posterior $p(w|\mathcal{D})$ is of the same form as the prior (example, both Gaussian).

For Bayesian linear regression, where $p(y|x) = \mathcal{N}(\mu = xw, \sigma^2)$, the conjugate prior is in fact the prior used for ℓ_2 regularization: $p(w) = \mathcal{N}(0, \sigma^2/\lambda)$. Given this prior, with prior mean $\mu_0 = 0$ and prior variance $\sigma_0^2 = \sigma^2/\lambda$, it can be derived that

$$
p(w|\mathcal{D}) = \mathcal{N}(\mu_n, \sigma_n^2) \qquad \text{where} \qquad
\begin{aligned}
\sigma_n^2 &= \frac{\sigma^2}{\sum_{i=1}^{n} x_i^2 + \lambda} \\
\mu_n &= \frac{\sum_{i=1}^{n} x_i y_i + \lambda\mu_0}{\sum_{i=1}^{n} x_i^2 + \lambda} = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2 + \lambda} = \frac{\sigma_n^2}{\sigma}\sum_{i=1}^{n} x_i y_i
\end{aligned}
$$

The MAP solution corresponds to the mode of this distribution: μ_n. Additionally, we can obtain a credible interval for which weights are plausible given the data, based on the variance σ_n. If the variance is big, then even after seeing the data there are many plausible values for w. As n gets larger, notice that σ_n^2 shrinks.

For linear regression, though, we typically have multivariate inputs and do not know the variance σ^2. Fortunately, even when extending more generally to this setting, we have a conjugate prior. First consider the univariate case. We need now a prior on weights $w \in \mathbb{R}$ and also the variance σ^2. The conjugate prior is called the Normal-Inverse-Gamma (NIG) distribution, which has four parameters: $\mu_n, \lambda_n, \alpha_n, b_n$. For prior parameters $\mu_0 \in \mathbb{R}$ and $\lambda_0, \alpha_0, b_0 > 0$ (e.g., $\mu_0 = 0, \lambda_0 = 0.1, \alpha_0 = 3, b_0 = 10$), we get posterior

$$p(w, \sigma^2|\mathcal{D}) = \text{NIG}(\mu_n, \lambda_n, a_n, b_n) \qquad \text{where} \quad \begin{aligned} \lambda_n &= \sum_{i=1}^n x_i^2 + \lambda \\ \mu_n &= \frac{\sum_{i=1}^n x_i y_i + \lambda_0 \mu_0}{\sum_{i=1}^n x_i^2 + \lambda} = \frac{\sum_{i=1}^n x_i y_i + \lambda_0 \mu_0}{\lambda_n} \\ a_n &= a_0 + \tfrac{1}{2} n \\ b_n &= b_0 + \tfrac{1}{2}\left(\sum_{i=1}^n y_i^2 + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2\right) \end{aligned}$$

For the NIG, the mode of the distribution is $\mathbb{E}[(w, \sigma^2)] = (\mu_n, \frac{b_n}{a_n - 1})$. The solution for w is the same as for MAP above. And now we also have an estimate for the most likely value for the variance of the noise $\frac{b_n}{a_n-1}$.

The solution for the variance is not that intuitive as given, but for certain settings it is more intuitive. Let's assume that the data is centered, meaning $\frac{1}{n}\sum_{i=1}^n x_i = 0$. Let's further assume simple choice on the prior parameters, $a_0 = 1, b_0 = 0$ and $\mu_0 = 0$, and use $\lambda = 0$ to minimally restrict the the solution for w, giving $\lambda_0 = 0$. For this setting, $\mu_n = w_{\text{MLE}} = \frac{\sum_{i=1}^n x_i y_i}{\sum_{i=1}^n x_i^2}$. Let $\hat{y}_i = w_{\text{MLE}} x_i$. Then we get that

$$\begin{aligned} \frac{b_n}{a_n - 1} &= \frac{b_0 + \frac{1}{2}\left(\sum_{i=1}^n y_i^2 + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2\right)}{a_0 + \frac{1}{2} n} \\ &= \frac{\frac{1}{2}\left(\sum_{i=1}^n y_i^2 - \lambda_n \mu_n^2\right)}{\frac{1}{2} n} && \triangleright\ \mu_n = w_{\text{MLE}} \\ &= \frac{\sum_{i=1}^n y_i^2 - w_{\text{MLE}} \lambda_n \mu_n}{n} && \triangleright\ \lambda_n \mu_n = \lambda_n \frac{\sum_{i=1}^n x_i y_i + \lambda_0 \mu_0}{\lambda_n} = \sum_{i=1}^n x_i y_i \\ &= \frac{1}{n}\left(\sum_{i=1}^n y_i^2 - w_{\text{MLE}} \sum_{i=1}^n x_i y_i\right) \\ &= \frac{1}{n}\sum_{i=1}^n (y_i^2 - w_{\text{MLE}} x_i y_i) \\ &= \frac{1}{n}\sum_{i=1}^n (y_i^2 - \hat{y}_i y_i) \\ &= \frac{1}{n}\sum_{i=1}^n (y_i^2 - 2\hat{y}_i y_i + \hat{y}_i^2) - \frac{1}{n}\sum_{i=1}^n (\hat{y}_i^2 - \hat{y}_i y_i) \\ &= \frac{1}{n}\sum_{i=1}^n (y_i - \hat{y}_i)^2 - \frac{1}{n}\sum_{i=1}^n (\hat{y}_i^2 - \hat{y}_i y_i) \end{aligned}$$

The first term $\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$ is a sample average estimate of the variance σ, using $\hat{y}_i$ as an estimate of $\mathbb{E}[Y|x_i]$. The second term reflects the additional variance due to the observed features themselves and the covariance between X and Y. The term $\frac{1}{n}\sum_{i=1}^{n}\hat{y}_i^2$ is a sample average estimate of the variance of the prediction, because an estimate of the variance is given by $\frac{1}{n}\sum_{i=1}^{n}\hat{y}_i^2 - (\frac{1}{n}\sum_{i=1}^{n}\hat{y}_i)^2$ and

$$\begin{aligned}\frac{1}{n}\sum_{i=1}^{n}\hat{y}_i &= \frac{1}{n}w_{\text{MLE}}\sum_{i=1}^{n}x_i \\ &= w_{\text{MLE}}\frac{1}{n}\sum_{i=1}^{n}x_i = 0\end{aligned}$$

because the data is centered, i.e., $\frac{1}{n}\sum_{i=1}^{n}x_i = 0$. This variance is subtracted from the noise variance estimate, because we want to remove the influence of the feature variance on our estimate of the noise variance. The second term $\frac{1}{n}\sum_{i=1}^{n}-\hat{y}_i y_i$ is a sample covariance between the prediction and the observed target. This covariance needs to be added to the above, to account for the fact that $\hat{y}_i$ is not an independent estimate of $\mathbb{E}[Y|x_i]$—it is correlated with y_i because it uses that data to get the estimate.

Now we can see how to maintain a distribution over w and the noise variance σ. The next step is to further generalize, to vector weights $\mathbf{w}$. The updates are similar to above, but require matrix inversions, so we leave them for a future course.

Chapter 12

Generalization Bounds

Note: This chapter is optional reading.

In this chapter, we provide theoretical 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). 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].

12.1 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 $\mathcal{F}$ to minimize a loss function $\ell : \mathbb{R} \times \mathbb{R} \to [0, \infty)$ in expectation over all pairs $(\mathbf{x}, y)$

$$\min_{f \in \mathcal{F}} \mathbb{E}[\ell(f(\boldsymbol{X}), Y)].$$

For example, in linear regression, $\mathcal{F} = \{f : \mathbb{R}^d \to \mathbb{R} \mid f(\mathbf{x}) = \mathbf{x}^\top \mathbf{w}, \text{ for any } \mathbf{w} \in \mathbb{R}^d\}$. This space of functions $\mathcal{F}$ 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 $\mathcal{F}$, where $\mathcal{F} = \{f : \mathbb{R}^d \to \mathbb{R} \mid f(\mathbf{x}) = \mathbf{x}^\top \mathbf{w}, \text{ for any } \mathbf{w} \in \mathbb{R}^d \text{ such that } \|\mathbf{w}\|_2 \le B_w\}$ for some finite scalar $B_w > 0$. Assume the input features come from a bounded space, such that for all $\mathbf{x}$, $\|\mathbf{x}\|_2 \le B_x$ for some finite scalar $B_x > 0$, and further that the outputs $y \in [-B_y, B_y]$ for some $B_y > 0$. Assume we use loss $\ell(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$, which is (locally) Lipschitz continuous for our bounded region, with Lipschitz constant $c = B_y + B_x B_w$. This is because $|\hat{y}| \le B_x B_w$ and

$$\left|\frac{d\ell(\hat{y}, y)}{d\hat{y}}\right| = |\hat{y} - y| \le |\hat{y}| + |y| \le B_y + B_x B_w.$$

Further, because $y \in [-B_y, B_y]$, we know the loss is bounded as

$$\ell(\hat{y}, y) = \tfrac{1}{2}(\hat{y} - y)^2 \leq \tfrac{1}{2}(B_y^2 + B_x^2 B_w^2).$$

For approximate error

$$\widehat{\mathrm{Err}}(f) = \frac{1}{n}\sum_{i=1}^{n} \ell(f(\mathbf{x}_i), y_i)$$

and true error

$$\mathrm{Err}(f) = \mathbb{E}[\ell(f(\boldsymbol{X}), Y)] = \int_{\mathcal{X}\times\mathcal{Y}} p(\mathbf{x}, y)\ell(f(\mathbf{x}), y)d\mathbf{x}dy$$

using Equation 12.2 below, we get that with probability $1 - \delta$, for $\delta \in (0, 1]$,

$$\mathrm{Err}(f) \leq \widehat{\mathrm{Err}}(f) + \frac{2cB_xB_w}{\sqrt{n}} + \tfrac{1}{2}(B_y^2 + B_x^2 B_w^2)\sqrt{\frac{\ln(1/\delta)}{2n}}. \tag{12.1}$$

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] For the linear functions above, with bounded ℓ_2 norms for $\mathbf{x}$, $\mathbf{w}$, the Rademacher complexity is bounded as $R_n(\mathcal{F}) \leq B_xB_y/\sqrt{n}$ (see [10, Equation 3]).

In the next few sections, we provide a generalization result for more general functions, as well as required background to determine that result.

12.2 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]

$$\hat{R}_n(\mathcal{F}) = \mathbb{E}\left[\max_{f\in\mathcal{F}} \frac{1}{n}\sum_{i=1}^{n} \sigma_i f(\mathbf{x}_i)\right]$$

[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.

[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 $\mathcal{F}$ 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 $[0, 1)$).

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 12.3.

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 $\sqrt{\frac{2\text{VC-dimension} \ln n}{n}}$.

12.3 Generalization Bound for General Function Classes

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 $f \in \mathcal{F}$,

$$\mathbb{E}[\ell(f(\boldsymbol{X}), Y)] \leq \frac{1}{n} \sum_{i=1}^{n} \ell(f(\mathbf{x}_i), y_i) + 2cR_n(\mathcal{F}) + b\sqrt{\frac{\ln(1/\delta)}{2n}} \tag{12.2}$$

For a more precise theorem statement and a proof, see [3, Theorem 7] and [10, Theorem 1].

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