Chapter 3

Probability and Information Theory

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

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

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

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

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

3.1 Why Probability?

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

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

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

There are three possible sources of uncertainty:

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

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

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

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

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

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

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

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

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

3.2 Random Variables

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

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

3.3 Probability Distributions

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

3.3.1 Discrete Variables and Probability Mass Functions

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

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

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

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

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

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

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

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

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

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

so the distribution is properly normalized.

3.3.2 Continuous Variables and Probability Density Functions

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

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

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

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

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

3.4 Marginal Probability

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

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

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