# Basic Probability and Statistics

Philip Schulz
Christian Schaffner

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# Contents

## Contributors

While we strive to continuously update this script and keep it on an acceptable level of grammaticality and mathematical correctness, it is unavoidable that some mistakes creep in. We are therefore utterly grateful to our contributors who have helped improving the script and would like to acknowledge their contributions here.

- Philip Michgelsen has corrected a mistake in the definition of event spaces in chapter 1.

# Chapter 1

# Basic Probability And Combinatorics

## Notational conventions

In this script we make use of certain notational conventions. We **bold-face** newly introduced technical terms on first mention. Those are the terms whose definitions you are expected to know by heart in this and following courses. *Italics* serve the purpose of highlighting passages in the script but also to discriminate linguistic examples from the rest of the text. Occasionally, we will point to online references outside of this script. The corresponding links are coloured in blue and you are encouraged to click them.

We denote sets with uppercase letters and overload notation by using $|\cdot|$ as both a function that yields the cardinality of a set and the length of a sequence. Besides using standard notation for set union and intersection we denote the complement of a set S with respect to another set X by $S\backslash X$.

## 1.1 Introduction

### 1.1.1 Why study probability theory?

The fact that you have picked up this script and started reading it demonstrates that you already have some interest in learning about probability theory. This probably means that you also have some conception of what probability theory is and what to do with it. Nevertheless, we will take the opportunity to quickly give you some additional motivations for studying probability theory.

This script is all about formalizing the notion of probability. In particular, we are interested in giving a formal interpretation to statements like "A is more probable than B". Let us take a simple example to demonstrate why this is useful: Suppose it is Monday and you have a date scheduled for Friday. Obviously you want to impress your date. Unluckily, however, you have tendency to be broke come weekends. The decision you have to make now is whether to take your date to a fancy restaurant (the impressive but expensive option) or to just go for drinks (the cheaper option). On what basis can you make this decision? Well, you can ask yourself whether it is more likely that you are broke on Friday night or not. If you think that you being broke is more probable than you going for drinks, otherwise you opt for the fancy restaurant.

The above is an example where we have used the intuitive notion of probability to assist us in decision making. The first part, the computation of the probabilities of events (e.g. you being broke or not) is something that we are going to develop in some detail in this script. The second part, the development of a so-called *decision rule* (e.g. to plan for the circumstances that are most probable to occur in the future) is something that will be covered in later courses.

Here is a second example of what one can do with probability theory. Assume you want to invest in the stock market. You will be putting in some money now and then you want to cash in on your gains (or losses) in ten years time, say. Notice that this time around simply asking whether it is more probable that your stock has risen or fallen in price is not enough. Even if your stock is worth more in ten years than it was when you bought it, the absolute increase may be so miniscule that you could have found much better investment options that would have yielded more gains. Worse even, if your gain is a smaller percentage of your original capital than the overall inflation that occurred during the ten years of your investment, you will actually have incurred a loss in terms of pure market power! So instead of asking whether or not your stock will be worth more than what it was when you first bought it, you should rather ask how much of an absolute gain you can expect from your investment. This second application of probability theory, the computation of expectations over real values, is something we are going to cover in this script, as well.

Alright, we hope that this has gotten you excited for the rest of the script. Let's get going!

## 1.2 Sample spaces and events

The whole of probability theory is based on assigning probability values to elements of a **sample space**. The members of the sample space are referred to as **outcomes** or **samples**.

**Definition 1.1 (Sample Space)** *A sample space is any Borel set* $\Omega$*. We denote the members of a sample space by* $\omega \in \Omega$*.*

Standard examples of sample spaces are the flipping of a coin and the rolling of a die. Formally, the sample space of a die roll is $\Omega = \{1, 2, 3, 4, 5, 6\}$. The sample space of a coin toss would consist of heads and tails. However, it is often more convenient to represent outcomes numerically. In the context of this course, we will achieve this by imposing any total order on the sample space and then identifying the outcomes with the positions they occupy in the corresponding ordered list. In this spirit we let the sample space of a coin toss be $\Omega = \{1, 2\}$ where 1 represents heads and 2 represents tails, say (the other way around would be just as fine).

More generally, we denote a sample space with $n$ members as $\Omega = \{1, \ldots, n\}$. A useful metaphor that we will often use is to think of generating an outcome from a sample space as a blind draw from an urn with $n$ balls that are numbered and possibly coloured but otherwise indistinguishable. The rolling of a die, for example, corresponds to drawing a ball from an urn with balls numbered 1 to 6. A somewhat more involved example is that of writing an English sentence of six words, for example the sentence: *To be or not to be.* The process of writing this sentence can be conceptualized as drawing six balls from an urn that contains balls corresponding to words in the English language[1]. Note that this will be a rather large urn as the vocabulary of the English language has already exceeded 1 million words.

In our sample spaces as defined above, it is easy to distinguish individual outcomes. However, often times we do not care about the outcomes themselves but about properties that some of them share. In the die example we might be only interested in whether the outcome is even or odd. Transferring this scenario to the urn metaphor we would colour the balls with odd numbers green and the balls with even numbers red. Again, any other colours are just as fine. All that matters is that we can discriminate a member of $E = \{2, 4, 6\}$ from a member of $O = \{1, 3, 5\}$. We do *not* need to discriminate between the outcomes that are members of the same set! In this particular setting $E$ and $O$ are the **events** that we are interested in.

**Definition 1.2 (Event)** *An event $A$ is any subset $A \subseteq \Omega$.*

Events are what usually interests us in probability theory. Just as with outcomes, we can also define the notion of an event space.

[1] This is obviously a very unrealistic conception of how English sentences are written as it totally ignores the fact that the words in a sentence are dependent on each other and have to be placed in a particular order.

**Definition 1.3 (Event space)** *An event space associated with a sample space $\Omega$ is a set $\mathcal{A}$ such that*

1. *$\mathcal{A}$ is non-empty*
2. *If $A \in \mathcal{A}$ then $A \subseteq \Omega$*
3. *If $A \in \mathcal{A}$ then $\Omega \setminus A \in \mathcal{A}$*
4. *If $A, B \in \mathcal{A}$ then $A \cup B \in \mathcal{A}$*

Notice that since $\emptyset \subseteq S$ for any set $S$ we always have $\Omega \in \mathcal{A}$ by item 3.

**Exercise 1.4** *You can also arrive at the conclusion that $\Omega \in \mathcal{A}$ always holds in a different (and arguably more cumbersome) way. How so?*

The fact that event spaces are closed under the set complement operation is very convenient. Say I organized a dinner party and invited 10 people. The day after you ask me if more than 8 people actually showed up. I just answer that I was very disappointed that my friends Mary and Paul did not come. Although I did not directly address your question you know that the answer is negative. After all, I informed you that the complement event of the event you asked about had occurred.

**Exercise 1.5** *In the above party example, what is the sample space? What is the smallest possible event space that is necessary to model the situation just described?*

In general, we will not worry too much about constructing an event space every time we encounter a new problem. The **power set** of the sample space conveniently happens to fulfil all the requirements we have for event spaces, so we will just always use it. Thus, all we will ever need to worry about is the construction of sample spaces since we now know how to construct event spaces from them in a simple manner. In case you are a bit rusty, here is a reminder of what a power set is.

**Definition 1.6 (Power Set)** *The power set $\mathcal{P}(S)$ of any set $S$ is defined as $\mathcal{P}(S) := \bigcup\limits_{s \subseteq S} s$.*

In general, this leaves us with the pair $(\Omega, \mathcal{P}(\Omega))$. For outcomes in a sample space, let us stress again an important difference, namely that $\omega \in \Omega$ but $\{\omega\} \in \mathcal{A}$.

## 1.3 Some basic combinatorics

Combinatorics is the mathematics of counting. Counting is of course a very basic problem that may be solved by just looking at each element of a set. However, this naïve procedure is often unreasonably time consuming. Moreover, it does not allow us to make general statements about sets of any size, i.e. sets of size $n$.

In order to assess the size of our sample spaces, we would like to make such general statements. The reason is that when we are dealing with probability we often start from **uniform probabilities** on the sample space where by uniform probability we simply mean the value $\frac{1}{|\Omega|}$. This is the probability we will assign to each and every $\omega \in \Omega$. We now say that all the elements in our sample space are equally probable. Note that at this point we are using probabilities solely for the purpose of motivating combinatorics which is kind of a hack because we haven't even told you yet what a probability is. However, we hope that you find the idea of uniform probabilities somewhat intuitive.

Let us start from scratch: What is the cardinality (size) of the sample space of a die roll? It is 6 because $|\{1, 2, 3, 4, 5, 6\}| = 6$. Now what if we roll two dice? The sample space for each individual die is already known. Let us call it $\Omega_1$. The sample space for the rolling of two dice is then just the Cartesian product of two such sample spaces, i.e. $\Omega_2 = \Omega_1 \times \Omega_1 = \{(x, y)|x \in \Omega_1, y \in \Omega_1\}$. Since the cardinality of the Cartesian product of two sets $S$ and $S'$ is $|S| \times |S'|$ we conclude that $|\Omega_2| = |\Omega_1 \times \Omega_1| = |\Omega_1| \times |\Omega_1| = |\Omega_1|^2 = 36$.

Unsurprisingly, this method of performing a draw from the same sample space (urn) multiple times generalizes to any number of times $n > 2$. Nicely enough, it also generalizes to sets of different sizes (again by the Cartesian product argument from above). However, we have to impose one important restriction on the use of this technique: it may only be applied when the sample spaces are independent, i.e. when the outcome of one space does not affect the outcome of the other. Often times, we will simply assume that this is the case, though.

The technique of inferring the size of a complex sample space from the sizes of the sample spaces it is constructed from is known as the **basic principle of counting**.

**Definition 1.7 (Basic principle of counting)** *The basic principle of counting states that if two draws from sample spaces of size $M$ and $N$ respectively are performed independently of each other then the sample space composed from them has size $M \times N$.*

**Exercise 1.8** *Let us assume that a football game is played for strictly 90 minutes. Both teams start with 11 players. A red card to a player results in that player being sent off the pitch. According to the rules of football, the game is stopped prematurely when either team has only 6 or fewer players remaining on the pitch. We are now interested in how many possible situations (we assume that situations occur in one-minute* *intervals) there are in which the game still progresses, one or more red cards have been issued and exactly four goals have been scored. Give the corresponding sample space and its size.*

Note that up to now we have implicitly assumed that we would put every drawn ball back into the urn. This is also referred to as **sampling with replacement**. Let us now look at problems for **sampling without replacement**, i.e. problems where we are shrinking our sample space at each draw. One class of such problems is known as **permutation** problems.

**Definition 1.9 (Permutation)** *A permutation on a set $S$ is a bijection $\sigma : S \to S : s \mapsto \sigma(s)$.*

Often times people also use the word permutation to refer to the image of a set under a permutation. What we need permutations for in practice is the reordering of ordered sets (which we will call lists). For example the permutations of the list $L = (1, 2, 3)$ are:

- $\sigma_1 = \{1 \mapsto 1, 2 \mapsto 2, 3 \mapsto 3\}$ $\qquad \sigma_1(L) = (1, 2, 3)$
- $\sigma_2 = \{1 \mapsto 1, 2 \mapsto 3, 3 \mapsto 2\}$ $\qquad \sigma_1(L) = (1, 3, 2)$
- $\sigma_3 = \{1 \mapsto 2, 2 \mapsto 1, 3 \mapsto 3\}$ $\qquad \sigma_1(L) = (2, 1, 3)$
- $\sigma_4 = \{1 \mapsto 2, 2 \mapsto 3, 3 \mapsto 1\}$ $\qquad \sigma_1(L) = (2, 3, 1)$
- $\sigma_5 = \{1 \mapsto 3, 2 \mapsto 1, 3 \mapsto 2\}$ $\qquad \sigma_1(L) = (3, 1, 2)$
- $\sigma_6 = \{1 \mapsto 3, 2 \mapsto 2, 3 \mapsto 1\}$ $\qquad \sigma_1(L) = (3, 2, 1)$

The way to think about a permutation as a draw from an urn is to look at each of the positions in the list in turn and insert an element from $S$. Since a permutation is a bijection, we can only use each $s \in S$ exactly once. This is precisely what it means to sample without replacement. Once a ball is drawn, it is removed from the urn. Let us make this effect concrete in the above example. For position one we have three elements to choose from. Hence we are dealing with a sample space of size 3. Position two still leaves us 2 choices, giving us a sample space of size 2. Finally, the element in the last position is totally determined as we are dealing with a sample space of size 1.

Applying the basic principle of counting we now know that there are $3 \times 2 \times 1$ permutations of the list $(1, 2, 3)$. Incidentally, this proves our above example to be correct. More generally, if we have to reorder a list with $n$ distinct elements (or draw without replacement from an urn with $n$ numbered balls), there are $n \times (n - 1) \times \ldots \times 2 \times 1$ permutations. Since this is pretty painful to write down we introduce a more succinct notation, provided by the **factorial** function.

**Definition 1.10 (Factorial)** *The factorial $n!$ of a non-negative natural number $n \in \mathbb{N}$ is defined recursively as*

- $0! = 1$
- $k! = k \times (k-1)!$ *for* $0 < k \leq n$

From the above discussion we can now conclude that the number of permutations on a set or list of size $n$ is $n!$.

We can also define the notion of a k-permutation on a set $S$ of size $n$ such that $k < n$. This means we are still drawing without replacement but we do not fully empty the urn. The reasoning for how many of those k-permutations there are remains exactly the same. There are $n \times (n-1) \times (n-k+2) \times (n-k+1)$ such permutations (make sure you understand why!). In order to ease notation we can again sneak in the factorial through multiplying this number with 1 in disguise. Concretely, we write

$$\begin{aligned} & n \times (n-1) \times \ldots \times (n-k+2) \times (n-k+1) \times 1 \\ =& n \times (n-1) \times \ldots \times (n-k+2) \times (n-k+1) \times \frac{(n-k)!}{(n-k)!} \\ =& \frac{n!}{(n-k)!} \end{aligned}$$

for the number of k-permutations on a set of size $n$.

We will not see k-permutations all that often in this script but they constitute a helpful stepping stone to another concept that will be of crucial importance. Let us draw $k$ balls from an urn with $n$ balls where $k \leq n$ and disregard the order in which we draw them. A classical example of such a setting would be the lottery where you are only interested in the balls drawn but not in the order in which they were drawn. We already know that for a set of $k$ balls there are $\frac{n!}{(n-k)!}$ orders in which we can draw them, as this is a $k$-permutation on our urn. Now, though, we need to get rid off the different orderings. This is to say that we want to count each set of $k$ balls that we can draw only once and not once per permutation of it. Luckily, we know how many permutations of a set of size $k$ there are, namely $k!$. Thus we divide out this number of permutations, yielding $\frac{n!}{(n-k)! \times k!}$ as the number of possible ways to draw $k$ *different* balls from an urn with $n$ balls. At this point we should take a break and pat our own backs. After all, we have just derived one of the most important combinatorial formulas, which is known as the **binomial coefficient**.

**Definition 1.11 (Binomial co-efficient)** *The binomial coefficient $\binom{n}{k}$ is defined as*

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

*for $0 < n, 0 \leq k \leq n$. It counts the number of ways to sample $k$ distinct elements from a set with a total of $n$ elements without regard to the order in which they are drawn. For this reason, it is pronounced "n choose k".*

**Exercise 1.12** *In the German lottery you have to bet on a set of 6 numbered balls to be drawn out of a total of 49 balls. Assuming that each ball is equally likely to be drawn, what is the chance of an individual bet to win the jackpot? The Dutch lottery is slightly more involved. They also draw an additional coloured ball from 6 coloured balls. In order to win the jackpot you need to have the number-colour combination right. What is your chance here?*

The binomial coefficient will become crucially important later on. A common application, that you will see in this and other courses is counting the number of bit strings with certain properties. A bit is a variable that can take on values in $\{0, 1\}$. By the basic principle of counting there are $2^n$ bit strings of length $n$. How many bit strings of length 5 are there that contain exactly 3 ones? Well, there are $2^5 = 32$ bit strings of that length in total and $\binom{5}{3} = 10$ of them contain exactly three ones. Unsurprisingly, this is the same number of 5-bit strings with exactly 2 zeros. The moral lesson here is that $\binom{n}{k} = \binom{n}{n-k}$ as can be easily seen from the definition. Some other trivia about the binomial coefficient are that $\binom{n}{0} = \binom{n}{n} = 1$. Again, this follows directly from the definition. Somewhat trickier is the fact that $\binom{n}{1} = \binom{n}{n-1} = n$. Can you derive this?

We can straightforwardly generalize the idea of the binomial coefficient to choosing more than just one set of objects. This means that instead of just looking at red versus non-red balls, say, we now distinguish between all the colours in our urn. For our strings this means that we move away from bit strings to strings with large alphabets, e.g. strings written in the English alphabet (which has 26 letters). Let's say we have $r$ red, $b$ blue, $g$ green and $y$ yellow balls in our urn such that $n = r + b + g + y$ is the total number of balls in the urn. How many different colour sequences can we draw? Well, we first arrange the $r$ red balls in $r$ out of $n$ positions. This can be done in $\binom{n}{r}$ ways. We then place the $b$ blue balls in $\binom{n-r}{b}$ ways. Next, we place the $g$ green balls in $\binom{n-r-b}{g}$ ways. Finally, we place the remaining yellow balls deterministically in the remaining positions since $\binom{n-r-b-g}{y} = \binom{y}{y} = 1$. We compute the total number of arrangements as

$$\binom{n}{r}\binom{n-r}{b}\binom{n-r-b}{g}\binom{n-r-b-g}{y} = \tag{1.1}$$

$$\frac{n!}{r! \times (n-r)!} \times \frac{(n-r)!}{b! \times (n-r-b)!} \times \frac{(n-r-b)!}{g! \times (n-r-b-g)!} \times 1 = \tag{1.2}$$

$$\frac{n!}{r!b!g!y!} \tag{1.3}$$

Observe that the last equality follows because many of the factorials cancel and because we know that $n - r - b - g = y$. We have now worked with only four colours, but the general case follows directly by induction on the number of colours (with the binomial coefficient as base case). Thus, we can define the **multinomial coefficient**.

**Definition 1.13 (Multinomial co-efficient)** *The multinomial coefficient for choosing $k$ sets of objects with size $m_k$ from a total of $0 < n = \sum\limits_{i=1}^{k} m_i$ objects is*

$$\frac{n!}{\prod\limits_{i=1}^{k} m_i!}$$

## Further material

For a slow and thorough introduction to combinatorics, see Faticoni (2013): Combinatorics. At the ILLC, there is a biannual course on combinatorics, taught by Ronald de Wolf. Online, Princeton also offers a course on combinatorics.

# Chapter 2

# Axiomatic Probability Theory

## 2.1 Axioms of Probability

In the previous chapter, we have introduced sample spaces and event spaces. We would like to be able to express that certain events are more (or less) likely than others. Therefore, we are going to measure the probability of events in a mathematically precise sense.

**Definition 2.1 (Finite Measure)** *A* finite measure *is a function $\mu : \mathcal{S} \to \mathbb{R} : S \mapsto \mu(S)$ that maps elements from a countable set of sets $\mathcal{S}$ (formally a $\sigma$-algebra) to real numbers. Such a measure has the following properties:*

1. *$\mu(S) \in \mathbb{R}$ for $S \in \mathcal{S}$,*
2. *$\mu\left(\bigcup\limits_{i=1}^{\infty} S_i\right) = \sum\limits_{i=1}^{\infty} \mu\left(S_i\right)$ for disjoint sets $S_1, S_2, \ldots$ .*

Notice that we are restricting ourselves to finite measures here, i.e. the value of the measure can never be infinite. This restriction makes sense as probabilities are finite as well. Property 2 is known as *countable additivity.*

Let $S = \bigcup\limits_{i=1}^{n} S_i$ for some positive natural number $n$ and disjoint $S_i$ and $S_j = \emptyset$ for $j > n$. By countable additivity, we then get

$$\mu(S) = \mu(\bigcup_{i=1}^{\infty} S_i) = \mu\left(\bigcup_{i=1}^{n} S_i \cup \bigcup_{j=n+1}^{\infty} \emptyset\right) = \sum_{i=1}^{n} \mu(S_i) + \sum_{j=n+1}^{\infty} \mu(\emptyset) \tag{2.1}$$

Since the $S_i$ are disjoint, we must have $\mu(S) = \sum\limits_{i=1}^{n} \mu(S_i)$ and it follows that $\mu(\emptyset) = 0$. We conclude that the empty set has measure 0 for all measures. Furthermore, we also see from the above derivation that countable additivity implies finite additivity, i.e. $\mu(S) = \sum_{i=1}^{n} \mu(S_i)$ for finite positive $n$ (again, this only holds if the $S_i$ are disjoint).

Examples of measures are not hard to find. In fact, we have already seen a measure, namely the function $|\cdot|$ that counts the elements of a set (check yourself that it really is a measure). Another measure is the Dirac-measure that is related to the characteristic function of a set. While the characteristic function tells you whether any object belongs to a given set, the Dirac-measure tells you whether any set contains a given object. Let us call the object in question $a$. Then its Dirac measure $\delta_a(S) = 1$ iff $a \in S$ and 0 otherwise (check yourself that the Dirac-measure indeed is a measure).

Apart from these examples, there is one measure, however, that is going to be the star of the rest of this script, namely the **probability measure**.

**Definition 2.2 (Probability measure)** *A probability measure* $\mathbb{P} : \mathcal{A} \to \mathbb{R}, A \mapsto \mathbb{P}(A)$ *on an event space* $\mathcal{A}$ *associated with a sample space* $\Omega$ *has the following properties:*

1. $\mathbb{P}(A) \geq 0$ *for all* $A \in \mathcal{A}$,
2. $\mathbb{P}\left(\bigcup_{i=1}^{\infty} A_i\right) = \sum_{i=1}^{\infty} \mathbb{P}(A_i)$ *for disjoint events* $A_1, A_2, \ldots$ ,
3. $\mathbb{P}(\Omega) = 1$ .

Notice that we only added Property 3 to the general definition of a measure. Hence, a **probability** (the value that the probability measure assigns to an event) will always lie in the real interval $[0, 1]$. The above three axioms for a probability measure are often referred to as *axioms of probability* or *Kolmogorov axioms* after their inventor Andrey Kolmogorov.

We have already discussed uniform probabilities in the previous chapter. We can now formally explain what we meant by that. The uniform probability measure $\mathbb{P}$ has the property that $\mathbb{P}(\{\omega\}) = \frac{1}{|\Omega|}$ for all $\omega \in \Omega$. At this point, the distinction between sample and event spaces becomes important. We cannot measure the elements of a sample space, only the elements of an event space! Recall our convention that we will always assume that $\mathcal{A} = \mathcal{P}(\Omega)$ which obviously contains a singleton for each element in $\Omega$. Using this assumption, the uniform probability measure is indeed well-defined. Whenever we talk about *uniform probability*, we either mean the uniform probability measure or, more often, the real value $\frac{1}{|\Omega|}$ to which this measure uniformly evaluates.

In order to create a tight relationship between a sample space, an event space and a probability measure, we introduce the concept of a **probability space**. Probability spaces are also known as **(probabilistic) experiments**.

**Definition 2.3 (Probability space)** *A probability space is a triple* $(\Omega, \mathcal{A}, \mathbb{P})$*, consisting of a sample space* $\Omega$*, an event space* $\mathcal{A}$ *and a probability measure* $\mathbb{P}$*.*

If we roll a die, for example, we have the sample space $\Omega = \{1, 2, 3, 4, 5, 6\}$ and, by convention, the event space $\mathcal{A} = \mathcal{P}(\Omega)$. If we add the uniform probability measure, we have constructed a *probabilistic experiment.* We can use it to answer a couple of questions. For example, we might wonder about the probability of obtaining an even number. By Property 2 of our definition, this probability is given by

$$\mathbb{P}(\{2, 4, 6)\}) = \mathbb{P}(\{2\} \cup \{4\} \cup \{6\}) \tag{2.2}$$

$$= \mathbb{P}(\{2\}) + \mathbb{P}(\{4\}) + \mathbb{P}(\{6\}) = \frac{1}{6} + \frac{1}{6} + \frac{1}{6} = \frac{1}{2} \tag{2.3}$$

Notice that this calculation is rather cumbersome. After all, we might just have evaluated $\mathbb{P}(\{2, 4, 6\})$ directly. This is because by convention we have $\mathcal{A} = \mathcal{P}(\Omega)$ which certainly contains $\{2, 4, 6\}$. Since the probability measure is defined on $\mathcal{A}$, it must map $\{2, 4, 6\}$ to some real number. However, the above calculation points to an interesting fact. In order to fully specify a probability measure, is suffices to specify the measure on the singleton sets of the event space. By countable additivity, this assignment already specifies the measure on the entire event space, as we can construct any event as a countable union of singletons.

It is important to point out that we just chose the uniform probability measure as the one that seems "natural" for a die roll. However, nobody is forcing us to do so. In fact, Definition 2.3 allows us to impose arbitrary probability measures.

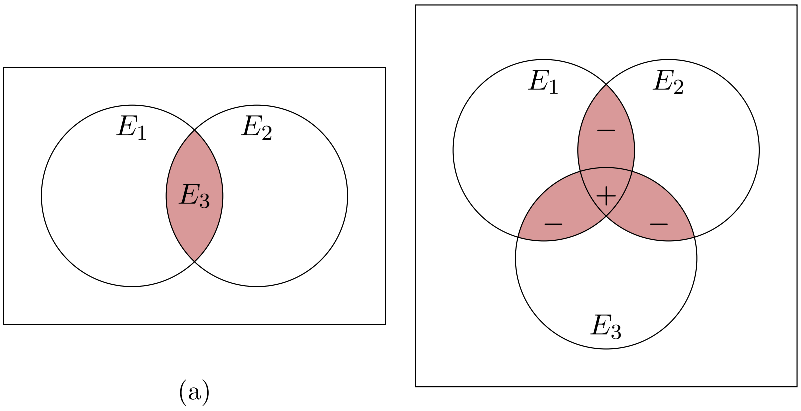
**Exercise 2.4** *Let us consider a rigged die. Take* $(\Omega, \mathcal{A}, \mathbb{P})$ *with* $\Omega$ *and* $\mathcal{A} = \mathcal{P}(\Omega)$ *as in the uniform die-roll example before, but use the probability measure specified by*
$\mathbb{P} = \{(\{1\}, 0), (\{2\}, \frac{1}{12}), (\{3\}, \frac{1}{6}), (\{4\}, \frac{1}{6}), (\{5\}, \frac{1}{3}), (\{6\}, \frac{1}{4})\}$.

1. *Verify that* $\mathbb{P}$ *is indeed a probability measure.*

2. *Compute the probability of obtaining a number strictly smaller than* $5$ *in this experiment.*

## 2.2 Probability of Arbitrary Unions of Events

We have seen how to compute probabilities of events if they can be formed as unions of *disjoint* events. The natural question to ask is what to do if we want to compute the probability of the *union of non-disjoint events.* In order to reason about this problem, we first take a step back and think



(a)

(b)

Figure 2.1: 2.1a: Two overlapping events $E_1$ and $E_2$. Their intersection (the coloured region) gets counted twice if we add up their probabilities.
2.1b: Venn diagram with 3 events. First we deduct $E_1 \cap E_2, E_1 \cap E_3, E_2 \cap E_3$ in order to prevent double counting and then we add in $E_1 \cap E_2 \cap E_3$. Deductions and additions are indicated by pluses and minuses.

about the outcomes of our probability space. We know that each event with non-zero probability contains at least one outcome (since $\mathbb{P}(\emptyset) = 0$, we can safely ignore the empty event). Let us assume that we take the union of events $E_1$ and $E_2$ with $E_1 \cap E_2 = E_3 \neq \emptyset$. This means that the outcomes in $E_3$ are contained in both $E_1$ and $E_2$. This situation is illustrated in Figure 2.1a. If we were to simply add up the probabilities of $E_1$ and $E_2$, we would effectively count the contribution of the outcomes in $E_3$ twice. We would hence get an overestimate of the actual value of $\mathbb{P}(E_1 \cup E_2)$. In order to avoid this we will need to subtract the probability of $E_3$ one time. This leads us to the following formulation:

$$\mathbb{P}(E_1 \cup E_2) = \mathbb{P}(E_1) + \mathbb{P}(E_2) - \mathbb{P}(E_1 \cap E_2) \tag{2.4}$$

Notice that this is fully general in that it is true even if $E_1$ and $E_2$ were disjoint. In that case, their intersection would be empty. We can generalize this principle to the (countable) union of an arbitrary number of events. This will give us a principled way of calculating the probability of any union of events. This calculation technique is know as the **Inclusion-Exclusion principle**.

**Theorem 2.5 (Inclusion-Exclusion principle)** *The probability of any (countable) union of events $E_1, \ldots, E_n$ can be computed as*

$$\mathbb{P}\left(\bigcup_{i=1}^{n} E_i\right) = \sum_{i=1}^{n}(-1)^{i+1}\left(\sum_{j_1<\ldots<j_i} \mathbb{P}\left(E_{j_1} \cap \ldots \cap E_{j_i}\right)\right) \tag{2.5}$$

We are going to proceed with a combinatorial proof of the Inclusion-Exclusion principle. It is very elegant but invokes the binomial theorem. For completeness sake we will prove the binomial theorem at the end of this chapter. For now, just trust us that it exists and is correct.

**Proof** We are going to focus on a particular outcome $\omega$ that is contained in $m$ events which we call without loss of generality $E_1, \ldots, E_m$ for some $m < n$. Notice that we can safely neglect all events which do not contain $\omega$, since $\omega$ is not going to contribute to their probability.

For all the $E_i$, $1 \leq i \leq m$ in which $\omega$ is contained, it is certainly true that $\omega$ is also contained in their intersections. The Inclusion-Exclusion-principle adds up or subtracts the probabilities of intersections of a given size. Notice that any intersection of more than $m$ events will not contain $\omega$ as we intersect with at least one event that does not contain $\omega$. Thus, we only need to consider intersections of our $m$ $\omega$-containing sets.

When $i = 1$ the intersection is trivial, as it just consists of one event. How many ways are there to pick one out of $m$ events? The answer is $\binom{m}{1}$. This is the number of times that $\omega$ contributes to the overall probability. At this point we have an overestimate of that probability (compare this to Figure 2.1a). Next we subtract the probabilities of the mutual intersections ($i = 2$). By the same reasoning as before, the contribution of $\omega$ is deducted $\binom{m}{2}$ times which gives us an underestimate since $\binom{m}{1} \leq \binom{m}{2}$ for $m \geq 3$. Since we are adding and subtracting in alternation, we will now keep flip-flopping between under- and over estimates. After considering all intersections of up to $m$ sets, we should get the correct result, however.

What we want to prove is that the right-hand side of (2.5) counts $\omega$'s contribution to the overall probability exactly once (because this is what happens on the left hand-side of (2.5)). That is, we have to prove that

$$1 = \sum_{i=1}^{m}(-1)^{i-1}\binom{m}{i} \tag{2.6}$$

We are right on our way towards exploiting the binomial theorem. Let us first state it.

$$(p+q)^m = \sum_{i=0}^{m}\binom{m}{i}p^i q^{n-i} \tag{2.7}$$

Setting $p = (-1)$ and $q = 1$, and multiplying both sides with $(-1)$, we obtain

$$-(-1+1)^m = -\sum_{i=0}^{n} \binom{m}{i} (-1)^i$$

which can be rewritten as

$$0 = -1 + \sum_{i=1}^{n} \binom{m}{i} (-1)^{i+1}\,, \tag{2.8}$$

because $\binom{m}{0} = 1$. Equation (2.8) implies (2.6) which we needed to prove. □

At this point we have done our fair share of math and found out how to calculate the probability of a union of events. We should ask ourselves what the probability of a union of events even tells us. Observe that an event occurs whenever we draw an outcome from our sample space that is contained in that event. By taking the union of events $E_1, \ldots, E_n$ we form a new event $E$ that (possibly) contains more outcomes than each of the original events. Thus, the probability of the $E$ will be higher than (or the same as) the probability of each of $E_1, \ldots, E_n$. What we are measuring then, is the probability that *any* of the events $E_1, \ldots, E_n$ occur. Crucially, we do not care anymore which one of them occurs.

What we are missing is a way to express the probability that a given number of events occur *together*. This concept is so important that we have a dedicated name for it, that of **joint probability**.

**Definition 2.6 (Joint probability)** *The joint probability of a (countable) set of events $\{E_1, \ldots, E_n\}$ is defined as*

$$\mathbb{P}(E_1 \cap \ldots \cap E_n)$$

*Sometimes one also finds the alternative notation*

$$\mathbb{P}(E_1, \ldots, E_n)$$

Wow, that was simple! We don not event need to prove another rule for calculating the joint probability. After all, we already know how to take the intersection of sets. Annoyingly, one problem remains: our definition of event spaces does not guarantee that they contain the intersections of their members. Or does it? Well, let us see whether we can “paraphrase” what an intersection is.

$$E_1 \cap E_2 = \Omega \backslash ((\Omega \backslash E_1) \cup (\Omega \backslash E_2)) \tag{2.9}$$

All the operations on the right hand side are defined for events spaces. We have thus solved our problem since we have shown that we can indeed do intersection in event spaces. To convince yourself that this is correct, you may want to consult Figure 2.1a. Alternatively, you may also just realise that this is an instance of DeMorgan's laws which you should know from set theory. Notice that we do not claim that this is the only valid "paraphrase". Feel free to find others, if you like!

## 2.3 Probability of Complements of Events

At this point we are capable to do most probabilistic computations that we will encounter in this course. From here on, it is all about making our lives easier. For example, how would you solve the following problem.

**Exercise 2.7** *You are observing a panel of 200 light bulbs and you know that at least one of them will light up once you press a button. What is the probability that any except the 87th bulb will light up? Note: this is a conceptual exercise. For the very keen ones, you can obtain the probability for each bulb to be turned on by typing the following into the Python interpreter:*

```
import numpy

probabilities = numpy.random.rand(1,200)
print probabilities/probabilities.sum()
```

The point of the above exercise is that it will be awfully cumbersome to compute the probability of the union of the singletons $E_i$ where $1 \leq i \leq 200$ and $i \neq 87$. On the other hand we can easily look up $\mathbb{P}(E_{87})$. The question is whether we can exploit this simpler calculation to help us answer the original question. Here we will again make use of the properties of event spaces. For any event $E$ in our event space we also have $\Omega \backslash E$ in the same space. Furthermore, $E$ and $\Omega \backslash E$ are disjoint which by our probability axioms means that we can simply add up their probabilities if we want to calculate the probability of their union. But what's the union of $E$ and $\Omega \backslash E$? It's exactly $\Omega$. From axiom 3 we know that $\mathbb{P}(\Omega) = 1$. By simple algebraic manipulations we find that

$$\mathbb{P}(\Omega \backslash E) = 1 - \mathbb{P}(E) \tag{2.10}$$

Thus if we want to find the probability that any but the $87th$ bulb will light up, we simply compute the probability that the $87th$ bulb will light up will light up and subtract that from 1. This is a rather general strategy to simplify calculations whenever the probability of an event is hard to compute. Maybe the probability of the complement of that event will be easier to compute.

**Exercise 2.8** *Show that in general*

$$\mathbb{P}(E_1 \backslash (E_1 \cap E_2)) = \mathbb{P}(E_1) - \mathbb{P}(E_1 \cap E_2)$$

## 2.4 Conditional Probability and Independence

After we have seen how to measure the probability of events, we are going to introduce another tremendously important concept, that of **conditional probability** measures.

**Definition 2.9 (Conditional probability measure)** *The probability of an event $E_i$ conditioned on another event $E_j$ with $\mathbb{P}(E_j) > 0$ is defined as*

$$\mathbb{P}(E_i|E_j) := \frac{\mathbb{P}(E_i \cap E_j)}{\mathbb{P}(E_j)}$$

Before we get into the math of conditional probabilities, let us try to understand the meaning of this concept. When we are computing the conditional probability of an event $E_i$, we re-scale with the probability of the conditioning event $E_j$. If $E_j \neq \Omega$, $\mathbb{P}(E_j)$ might be smaller than 1. Thus, this rescaling assumes *that $E_j$ has already occurred.* In other words, we are excluding all outcomes that are not in $E_j$ from further consideration (even though they may be in $E_i$). The interpretation of conditional probabilities is that they are the probabilities of events assuming that another event has already occurred.

Another interpretation is that when working with a conditional probability measure, we are in fact working in a new probability space, where $\Omega_{new} = E_2$, i.e. our new sample space is the conditioning event. Notice that this also means that our probability measure will change and become the measure from Definition 2.9.

Here comes the cool part: although we have introduced a new concept, all the properties of probability measures that we know by now will seamlessly carry over to conditional probabilities, if we can prove that the conditional probability measure is a probability measure according to our axioms.

**Exercise 2.10** *Use the axioms from Definition 2.2 to prove that $\mathbb{P}(\cdot|E_j)$ is a probability measure.*

We will make use of conditional probabilities quite a lot in this course. We will later see a way in which they help us to decompose joint probability distributions. For now, we are going to focus on the fact that they are also related to the idea of independence of events.

**Definition 2.11 (Independence)** *Two events $E_1, E_2$ are said to be independent if*

$$\mathbb{P}(E_1 \cap E_2) = \mathbb{P}(E_1) \times \mathbb{P}(E_2)$$

*Independence of two events is denoted as $E_1 \perp E_2$.*

This definition relates to conditional probabilities in the following way: assume that $E_1 \perp E_2$. Then we get

$$\mathbb{P}(E_1|E_2) = \frac{\mathbb{P}(E_1 \cap E_2)}{\mathbb{P}(E_2)} = \frac{\mathbb{P}(E_1) \times \mathbb{P}(E_2)}{\mathbb{P}(E_2)} = \mathbb{P}(E_1)\,. \tag{2.11}$$

Hence, independence of two events $E_1 \perp E_2$ is equivalent with $\mathbb{P}(E_1|E_2) = \mathbb{P}(E_1)$.

**Exercise 2.12** *Prove that $E_1 \perp E_2$ is also equivalent with $\mathbb{P}(E_2|E_1) = \mathbb{P}(E_2)$.*

Independence will prove to be a useful concept in later chapters. More precisely, we will often just *assume* that two events (or random variables – see the next chapter) are independent. Although such an independence assumption might not always hold in practice, it will allow us to formulate much simpler probabilistic models.

## 2.5 A Remark on the Interpretation of Probabilities*

This concludes our introduction of axiomatic probability theory. We know that a probability is a real number in $[0, 1]$. For all that we are going to do in this course (and in most follow-up courses) this is fully sufficient. However, some of you may wonder what a "natural" interpretation of probabilities would be. There are two dominating views on that. One postulates that if we were to take A LOT (read: almost infinitely many) samples from a sample space, the probability of an event is its frequency amongst these samples divided by the total number of samples taken. For those of you who know limits, this principle can be formalized as $\mathbb{P}(E) = \underset{n\to\infty}{lim} \frac{\#E}{n}$. This view is known as the *frequentist view.*

The second view postulates that probabilities are an expression for degrees of belief. Basically, if you assign $\mathbb{P}(E)$ to an event $E$, then $\mathbb{P}(E)$ is the strength of your personal belief that $E$ will occur. This latter view is known as the *Bayesian view.*

Which conception of probability you choose is a philosophical matter and does not really impact the math. That is why we will not care about this issue in this course. However, it is useful to at least be aware of these two views (if only to appear knowledgeable in a conversation you may have with your philosopher friends).

## 2.6 The Binomial Theorem

The binomial theorem from Equation 2.7 is actually not that hard to prove. We will do so by induction. As a base case we choose $m = 0$. Then the equality is easy to see.

$$(p+q)^0 = 1 = \binom{0}{0} p^0 q^0 \tag{2.12}$$

Next, we assume that the theorem holds for $m = n$. What we want to show is that it also holds for $m = n + 1$. We achieve this by algebraic manipulation.

$$\begin{align}
(p+q)^{n+1} &= (p+q)^n \times (p+q) \tag{2.13}\\
&= (p+q)^n p + (p+q)^n q \tag{2.14}\\
&= p\sum_{i=0}^{n} \binom{n}{i} p^i q^{n-i} + q\sum_{i=0}^{n} \binom{n}{i} p^i q^{n-i} \tag{2.15}\\
&= \sum_{i=0}^{n} \binom{n}{i} p^{i+1} q^{n-i} + \sum_{i=0}^{n} \binom{n}{i} p^i q^{n+1-i} \tag{2.16}\\
&= \sum_{j=1}^{n+1} \binom{n}{j-1} p^j q^{n+1-j} + \sum_{i=0}^{n} \binom{n}{i} p^i q^{n+1-i} \tag{2.17}\\
&= \binom{n}{n} p^{n+1} q^{(n+1)-(n+1)} + \sum_{k=1}^{n} \binom{n}{k-1} p^k q^{n+1-k} \tag{2.18}\\
&\quad + \binom{n}{0} p^0 q^{n+1} + \sum_{k=1}^{n} \binom{n}{k} p^k q^{n+1-k} \notag
\end{align}$$

$$= q^{n+1} + p^{n+1} + \sum_{k=1}^{n} \left( \binom{n}{k} + \binom{n}{k-1} \right) p^i q^{n+1-k} \tag{2.19}$$

$$= q^{n+1} + p^{n+1} + \sum_{k=1}^{n} \left( \frac{n!}{k!(n-k)!} + \frac{n!}{(k-1)!(n-k+1)!} \right) p^i q^{n+1-k} \tag{2.20}$$

$$= q^{n+1} + p^{n+1} + \sum_{k=1}^{n} \left( \frac{n!(n+1-k)}{k!(n+1-k)!} + \frac{n!k}{k!(n-k+1)!} \right) p^k q^{n+1-k} \tag{2.21}$$

$$= q^{n+1} + p^{n+1} + \sum_{k=1}^{n} \left( \frac{n!(n+1)}{k!(n+1-k)!} \right) p^i q^{n+1-k} \tag{2.22}$$

$$= q^{n+1} + p^{n+1} + \sum_{k=1}^{n} \binom{n+1}{k} p^k q^{n+1-k} \tag{2.23}$$

$$= \sum_{i=0}^{n+1} \binom{n}{k} p^k q^{n-k} \tag{2.24}$$

Let us clarify some parts of the proof. We use the induction hypothesis to expand the terms in Line 2.15. In Line 2.17, we switch the variable $i$ in the first summand to $j = i + 1$. The reason why we do this is because we want to achieve congruence with the exponents of the second summand. In the following line we uniformly name the variables $k$. Since $k$ has to run over a common range, we chop off the ends of both sums that stick out. In the first sum of line 2.17 that is the summand that corresponds to $j = n+1$ and in the second sum it is the summand that corresponds to $i = 0$. We pull out both of them in line 2.18 and then collapse the sums in line 2.19. The following lines are basically just an exercise in manipulation fractions. The jump from the second-to-last to the last line is allowed because

$$q^{n+1} = \binom{n+1}{0} p^0 q^{n+1-0}$$

and

$$p^{n+1} = \binom{n+1}{n+1} p^{n+1} q^{(n+1)-(n+1)}$$

which are exactly the quantities that we need to add to make our sum reach from 0 to $n+1$. This completes the proof.

## Further Reading

A very quick and dirty introduction to measure theory is provided by Maya Gupta and can be found here. If you are looking for something more extensive that also motivates event spaces and the like you may want to take a look at this script by Ross Leadbatter and Stamatis Cambanis (which has also been published as a book).

# Chapter 3

# Random Variables and Their Properties

## 3.1 What is a Random Variable?

**Random variables** are a tremendously useful concept in probability theory. In most situations of science and general life we are not really interested in the actual outcome of a random experiment. Instead, we care about particular properties of that outcome.

For starters, let us talk about the weather. Like most people living in the north of Europe, your choice of clothing probably depends strongly on the weather. Let us assume that you have a thick winter jacket that you put on when it is cold, a light soft-shell jacket that you wear when temperatures are mild and that you simply wear a T-shirt or a sweater when it is warm. Let us also assume that the forecasting site you consult every morning reports the temperatures up to one decimal. The question is: does it matter to you whether it is 5.4 or 7.3 degrees centigrade outside when you make your decision about what to wear? Most likely you are only interested in whether it is cold, mild or warm. This may obviously vary according to your own perception of warmth and cold. Here we will assume that it is cold whenever the temperature is below 10 degrees, mild between 10 and 20 degrees (inclusive) and warm whenever the temperature rises above 20 degrees. So what you are really interested in, at least as far as clothing is concerned, is whether the temperature $t$ is $t < 10$ or $10 \leq t \leq 20$ or $t > 20$. What we are looking for is a way of transforming outcomes from the temperature scale into judgements of perceived temperature.

Another example is the lottery. Let us again consider the German lottery where you have to correctly predict 6 out of 49 numbers all of which are drawn *independently* and *uniformly at random* (you should be able to understand the first term by now; after reading this chapter, you will also understand the second). You get the main prize if you predict all these items correctly. However, pay-outs start from three correctly predicted numbers and increase for each additional number that you got right. So what do you really care about when playing the lottery? Does it matter to you whether or not you correctly predicted the number 39? Probably not. All you care about is how many of the numbers you got right.

Observe that one possible way of modelling the sample space for the lottery situation is the following:

$$\begin{aligned}\Omega = \{(b_1, \ldots, b_6, c_1, \ldots, c_6) \,|1 \leq b_1 < b_2 < \ldots < b_6 \leq 49; \\ c_1, \ldots, c_6 \in \{0, 1\}\}\end{aligned} \tag{3.1}$$

This rather cumbersome expression states that we draw 6 balls from an urn of 49 balls without replacement (and then sort them). We also add indicators of whether we predicted each ball drawn correctly. Note that we did not model what exactly our prediction was, but only if we predicted a number correctly. So again the question arises of how we can transform outcomes from this sample space into the events that we actually care about (namely how many balls we predicted correctly)?

After this little motivating section, let us formally define what a random variable is.

**Definition 3.1 (Real random variable)** *A (real) random variable (RV) X on a probability space* $(\Omega, \mathcal{A}, \mathbb{P})$ *is a function*

$$X : \Omega \to \mathbb{R}$$

*where we require that for all* $r \in \mathbb{R}$*, the set* $A = \{\omega | X(\omega) \leq r\}$ *is in the event space* $\mathcal{A}$*.*

Notice that the naming of the random variable is arbitrary but by convention we will often use the capital letters $X, Y, Z$. Also, as you can see, RVs are defined on an entire probability space. The reason is that we want to have a probability measure associated with our sample space. In fact, this probability measure is the reason why we can see random variables as taking on their values in a random way. Moreover, since we can only measure events from our event space, the condition on RVs ensures that we can in fact measure the probability of each real value which a RV may map an outcome to. In technical terms, we are thus making sure that the pre-image of the RV is *measurable*.

Let us define a random variable for the weather situation.

$$X(t) = \begin{cases} 1 & t < 10\,, \\ 2 & 10 \leq t \leq 20\,, \\ 3 & t > 2\,. \end{cases} \tag{3.2}$$

In principle we can easily determine the probability of each of the values of this RV. However, we did not bother to define a sample space and associated probability measure, mostly because we would have to restrict the possible temperatures to those that we think are reasonable. Nevertheless, this is something that you can do yourself.

**Exercise 3.2** *Define an upper and lower bound for temperature values (make sure you can actually get all three perceived degrees of warmth). These bounds will lead you to a discrete sample space since we postulated that the website we consult only reports temperatures up to one decimal place after the comma. Then impose any probability measure on the associated event space. Finally, compute the probability of each of the values of the RV $X$ from Equation (3.2).*

We can do the same for the lottery. Our random variable would then look as follows:

$$X(\omega) = \sum_{i=1}^{6} c_i \tag{3.3}$$

Whenever a RV assumes a particular value, we write $X = x$. Thus, if $X$ in Equation (3.3) assumes the value 4, i.e. we guessed four balls correctly, we would write $X = 4$. And here comes the function that computes the probability that this event happens.

**Definition 3.3 (Probability distribution)** *The discrete probability distribution of a RV $X$ is denoted by $P_X$ and is defined as the function*

$$P_X(X = x) := \mathbb{P}(\, \{\omega \mid X(\omega) = x\} \,)$$

*In the literature, often one of the two mentions of $X$ is dropped from the notation, resulting in $P(X = x)$ or $P_X(x)$.*

What is $P(X = 4)$ for the lottery example? Recall that there are $a = \binom{49}{6}$ sequences of balls that we can draw (6 out of 49 balls). In our modelling of the scenario, we also have to take into account whether or not we correctly predicted each ball. Notice that the indicator $c_i$ is a function of our predictions. If our prediction $v_1, \ldots, v_6$ are ordered in ascending fashion, then

$$c_i = \begin{cases} 1 & \text{if } v_i = b_i \\ 0 & otherwise \end{cases}$$

The unfairness of the lottery comes from the fact that the player has to pick out of a large number of sequences only very few of which will have more than three numbers in common with the sequence that ends up being drawn. Let us apply this intuition to our example. There are $\binom{6}{4}\binom{43}{2}$ ways in which your predictions can get exactly 4 numbers right. This is because there are $\binom{6}{4}$ ways to guess 4 out of 6 numbers correctly and $\binom{43}{2}$ ways to choose any two out of the 43 numbers that were not drawn. In total there are

$$\binom{6}{4}\binom{43}{2} = 13545 \tag{3.4}$$

ways to agree on four balls with some lottery draw. This might seem like a lot. However, if we divide this by the total number of possible lottery draws, we find that $P(X = 4) = 0.000969$ which is very little.

We have just seen examples where the RV takes on a specific value. We can of course also make statements like $X < x$ and $X \geq x$. This is a way of expressing that a RV assumes a value above or below a certain threshold. The way to get the probability of this event is through the cumulative distribution function.

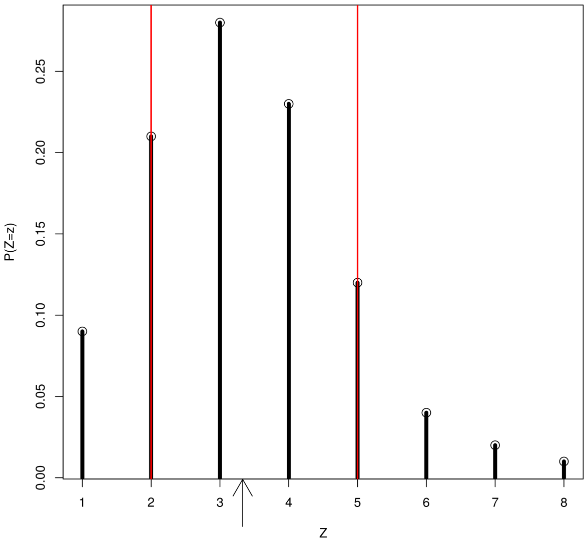


Figure 3.1: Probability distribution of a random variable $Z$ with 8 possible values, given by $P(Z=1)=0.09, P(Z=2)=0.21, P(Z=3)=0.28, P(Z=4)=0.23, P(Z=5)=0.12, P(Z=6)=0.04, P(Z=7)=0.02$, and $P(Z=8)=0.01$. The arrow indicates the expectation. This is a visualisation of the spike that we can plug underneath the centre of mass.

**Definition 3.4 (Cumulative distribution function)** *The* ***cumulative distribution function (cdf)*** *of a random variable $X$ is given by*

$$F_X(a) := P(X \leq a) = \sum_{x \leq a} P(X = x)$$

The cumulative distribution function is helpful in two ways. First of all, it allows to get the probability that $X$ takes on a value in a certain range. Second, it has applications in sampling algorithms, some of which we might see during the programming part of the course. A plot of the cdf of $Z$ is given in Figure 3.2. We can recognize that it is the cdf of a discrete distribution because it is discontinuous. If the underlying probability distribution was continuous, so would be its cdf.

To better understand how we can compute the probability that $a \leq X \leq b$ for some real values $a, b$ let us take a look at Figure 3.1. There we see a plot of the probability distribution of a random variable $Z$. The red lines indicate the interval that we are interested in. As a warm-up exercise, let us first compute $P(Z \leq 2)$ and $P(Z > 5)$. By looking at the plot we easily see which areas we need to consider, namely the bars to the left of 2 and to the right of 5. The height of the bars corresponds to their probability.

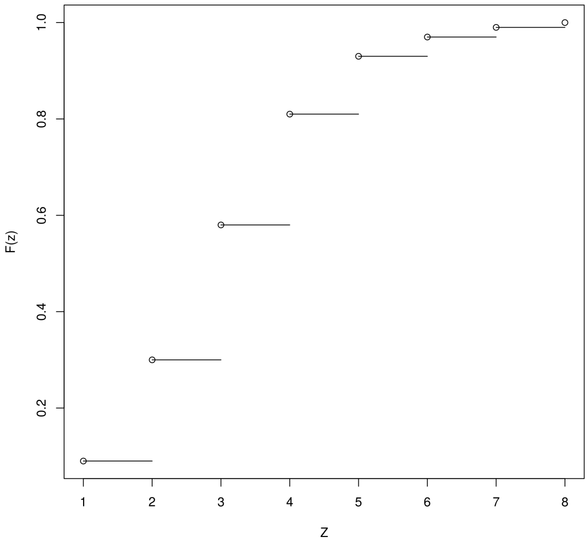


Figure 3.2: Cumulative probability distribution of $Z$. Observe that it stays constant in values that $Z$ cannot take on. This cdf being discontinuous is an indicator that the underlying probability distribution is discrete.

We go on to compute the probability that $Z$ is smaller or equal to 2 and that $Z$ is bigger or equal to 5:

$$P(Z \leq 2) = P(Z = 1) + P(Z = 2) = 0.09 + 0.21 = 0.3 \tag{3.5}$$

$$\begin{aligned} P(Z > 5) &= P(Z = 6) + P(Z = 7) + P(Z = 8) \\ &= 0.04 + 0.02 + 0.01 = 0.07 \end{aligned} \tag{3.6}$$

It is straightforward to compute $P(2 < Z \leq 5)$. If we again look at Figure 3.1, we see that this is the area delimited by the red lines. Thus, $P(Z \leq 5)$ will be an overestimate of this probability. The amount by which it is an overestimate is exactly $P(Z \leq 2)$. Thus we get $P(2 < Z \leq 5) = P(Z \leq 5) - P(Z \leq 2)$.

**Exercise 3.5** *We claim that you can compute $P(2 < Z \leq 5)$ based on $P(Z \leq 2)$ and $P(Z > 5)$ from above. What result do you get?*

In the case of discrete random variables, i.e. the ones that we are dealing with here, there is another function that is of great interest, namely the probability mass function.

**Definition 3.6 (Probability mass function)** *The **probability mass function (pmf)** of a random variable $X$ is given by*

$$p(x) := P(X = x)$$

The pmf is notationally more convenient than the probability distribution but also less general. For example, the pmf does not allow us to express that $X$ falls in a range of values. In order to avoid confusion, we will mostly use $X$'s probability distribution here. Be aware, however, that most papers that you are going to read in the future will use the pmf instead. Regardless of whether we are using the probability distribution or the pmf, we will call the values in $\mathbb{R}$ to which they assign positive probability, their support.

**Definition 3.7** *The **support** of a random variable $X$ is given by*

$$\operatorname{supp}(X) := \{x \in \mathbb{R} \mid P(X = x) > 0\}$$

## 3.2 Expectation and Variance

There are two major properties of probability distributions that are used to describe them. One is the center of mass, the point at which the probability mass of the distribution is split into half. If you think of the support of $P$ as a plank and of the probabilities as weights, then the center of mass is the point at which you could put an infinitely thin spike into the plank from underneath such that the plank maintains perfect balance. In Figure 3.1 this so-called expectation is indicated by an arrow that can be interpreted as visualising the spike that we can plug underneath the probability plank.

**Definition 3.8 (Expectation)** *The **expectation** of a random variable $X$ with respect to the distribution $P$ is defined as*

$$\mathbb{E}[X] := \sum_{x \in \operatorname{supp}(X)} x P(X = x)\,.$$

**Exercise 3.9** *Compute the expectation of the random variable $Z$ from the previous section.*

It is important to point out that the expectation of a random variable is a real number which does not need to in the support of $X$. This is for example the case in Figure 3.1 where the expectation is fractional although all support values are integers.

The expectation comes with an interesting property that is called the **linearity of expectation**. Basically, whenever we multiply $X$ with a constant $a$, the expectation will also be scaled by that constant. Moreover, when we add a constant $b$ to $X$ the expectation will also increase/decrease by $b$ (depending on whether $b$ is positive or negative). Let us prove that!

$$\mathbb{E}[aX+b] = \sum_{x\in\text{supp}(X)} (ax+b)P(X=x) \tag{3.7}$$

$$= a\sum_{x\in\text{supp}(X)} xP(X=x) \;+\; b\sum_{x\in\text{supp}(X)} P(X=x) \tag{3.8}$$

$$= a\mathbb{E}(X) + b \tag{3.9}$$

The equality in (3.9) follows from the fact that the sum of the probabilities of the support of a distribution is 1. The linearity of expectation is extremely useful. Basically, if you know the expectation of a RV you also know the expectation of its multiples. Furthermore, by adding a constant, we basically shift each element in the support. However, this shifting does not do anything surprising as the centre of mass shifts by the same amount.

We can actually take the expectation of any quantity, but it only has an effect on quantities that can be cast as functions of $X$. The expectation of a quantity that is constant with respect to $X$ will just be that quantity itself. More formally:

$$\mathbb{E}[b] = \sum_{x\in\text{supp}(X)} bP(X=x) = b \tag{3.10}$$

A class of functions of $X$ that people are often interested in are the moments. Moments are the powers of $X$, so $X$ itself is the first moment, $X^2$ is the second moment and so on. We will not further discuss moments here, but it is useful to at least know what they are in case you find the expression in a paper.

After we have discussed the centre of mass, it is also interesting to look at how far the outcomes are spread around the average. Assume two random variables $X$ and $Y$ with

- $P(X=-100)=0.5$; $P(X=100)=0.5$
- $P(Y=-1000)=0.5$; $P(Y=1000)=0.5$

The spread of $Y$ is obviously going to be greater, although both have the same expectation. The quantity usually used to assess the spread of a RV is the variance.

**Definition 3.10 (Variance)** *The variance of a RV X is given by*

$$\text{var}(X) := \mathbb{E}[\,(X-\mathbb{E}[X])^2\,]\,.$$

The expression for $\mathrm{var}(X)$ is rather scary-looking but let us try to make sense of it. The inner part is the difference between each value of the random variable and the expectation. Thus the outer expectation is just a weighted sum of differences between values in the support and the expectation. However, since values of $X$ can be smaller or greater than the expectation, this sum will be 0. Therefore we square it, leaving us with only positive values. In summary, the variance is the expectation of the squared differences between the expectation and the values in the support of $X$.

Computing the variance as an expectation can be cumbersome. We show how it can be done more efficiently.

$$\mathrm{var}(X) = \mathbb{E}[\,(X - \mathbb{E}[X])^2\,] \tag{3.11}$$

$$= \sum_{x \in \mathrm{supp}(X)} P(X = x)(x - \mathbb{E}[X])^2 \tag{3.12}$$

$$= \sum_{x \in \mathrm{supp}(X)} P(X = x)(x^2 - 2x\mathbb{E}[X] + \mathbb{E}[X]^2) \tag{3.13}$$

$$= \sum_{x \in \mathrm{supp}(X)} P(X = x)x^2 - \sum_{x \in \mathrm{supp}(X)} P(X = x)2x\mathbb{E}[X] + \mathbb{E}[X]^2 \tag{3.14}$$

$$= \mathbb{E}[X^2] - 2\mathbb{E}[X]^2 + \mathbb{E}[X]^2 \tag{3.15}$$

$$= \mathbb{E}[X^2] - \mathbb{E}[X]^2\,. \tag{3.16}$$

For most intents and purposes we will use (3.16) to compute the variance.

**Exercise 3.11** *Compute the variance of the RV $Z$ from the previous section.*

Although variance is not linear, we can still try to figure out what happens when we multiply a RV by a constant or add a constant to it.

$$\mathrm{var}(aX + b) = \mathbb{E}[(aX + b - \mathbb{E}[aX + b])^2] \tag{3.17}$$

$$= \mathbb{E}[(aX + b - a\mathbb{E}[X] - b)^2] \tag{3.18}$$

$$= \mathbb{E}[a^2(X - \mathbb{E}[X])^2] \tag{3.19}$$

$$= a^2\,\mathrm{var}(X) \tag{3.20}$$

**Exercise 3.12** *Give an alternative proof of* $\mathrm{var}(aX + b) = a^2\,\mathrm{var}(X)$ *by using* $\mathrm{var}(X) = \mathbb{E}[X^2] - \mathbb{E}[X]^2$.

What we see that the variance is not affected by adding a constant to the RV. This makes sense, as constant additions just shift the expectation. However, the relation of each individual value to the expectation is not affected by that operation. On the other hand, when we multiply each value of the RV by a constant, the variance is scaled by the square of that

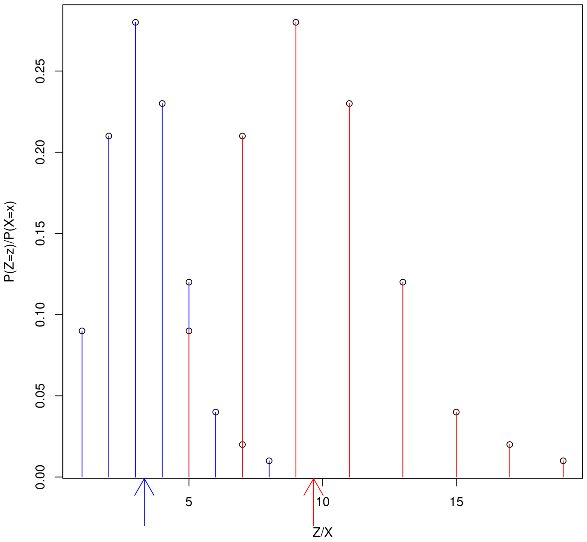


Figure 3.3: Plot of RVs $Z$ and $X = 2Z + 3$. The arrows indicate the expectation of each distribution.

constant. Again, this is not surprising. Remember that we used squaring in our definition of the variance to turn all distances from the expectation into positive numbers. If we multiply an RV by a constant $a$, its spread will increase in both directions by a factor of $a$. Since we again want only positive differences, we better square that increased spread. This intuitively justifies the above equalities.

To gain a visual understanding of what happens when a RV gets scaled and a constant gets added to it, take a look at Figure 3.3. The random variable $Z$ is the same as in Figure 3.1 and its probability distribution is plotted in blue. Figure 3.3 also shows the probability distribution of another RV $X = 2Z + 3$ in red. As predicted by our calculations above, the expectation (indicated by the red arrow) shifts by two times its original value plus three. Furthermore, note that the addition of three does not have any influence on the variance of $X$. The relative distance between the elements in the support of $X$ is the same as the relative distance between the elements in the support of $Z$. However, the distance between the smallest and largest value in the support has doubled, hence increasing the variance by a factor of $2^2 = 4$.

## 3.3 Joint and conditional distributions

Up to now, we have only looked at cases that could be treated with one random variable. Most interesting problems involve several RVs, however. We introduce the concept of jointly distributed random variables. What this means is that there is a distribution over tuples of values, each from a different RV.

**Definition 3.13 (Joint probability distribution)** *Random variables $X_1, \ldots, X_n$ (**abbreviated as** $X_1^n$) are said to be **jointly distributed** with probability distribution $P_{X_1^n}$ if*

$$P(X_1 = x_1, \ldots, X_n = x_n) = \mathbb{P}(\,\{\omega \mid X_1(\omega) = x_1, \ldots, X_n(\omega) = x_n\}\,)\,.$$

From the above definition, we see that the random variables need to share an underlying sample space. This also gives us more insight into the real power of RVs: in applications, we usually do not care at all about the underlying sample space but only about quantities captured by the RVs. Therefore, we define a probability distribution over the random variables of interest. Since by definition the distribution has to fulfil conditions that allow us to interpret the distribution as a probability measure on a probability space, we can use the distribution without worrying about the underlying sample space.

Joint distributions are of particular interest because they make it possible to recover the probability distribution of each individual RV as well as of smaller joint distributions. The process by which this recovery can be accomplished is known as **marginalization**. Say we are given a joint distribution $P_{XY}$. How can we determine the probability that $X = x$? Our sample space is carved up by the values that $X$ and $Y$ can take on. We are interested in the probability of the subset $E = \{\omega | X(\omega) = x\}$. Assuming that $Y$ can take on $n$ values $y_1, y_2, \ldots, y_n$, let us define $F_i = \{\omega | Y(\omega) = y_i\}$ for $1 \leq i \leq n$. Some (possibly all) of the $F_i$ will overlap with $E$. Thus we can partition $E$ into $E \cap F_1, \ldots, E \cap F_n$. By countable additivity, we simply need to sum up the probabilities of these intersections. Observe that those probabilities correspond exactly to $P(X = x, Y = y_1), \ldots, P(X = x, Y = y_1)$. Hence, we get to the following equality:

$$P(X = x) = \sum_{i=1}^{n} P(X = x, Y = y_i) \tag{3.21}$$

If we set $X = (Z_1, \ldots, Z_m)$, we can recover $P_{Z_1^m}$ from $P_{Z_1^m Y}$ in the same way. Likewise, if we set $Y = (Z_1, \ldots, Z_m)$ we get the generalization of (3.21). We will assume that each $Z_j$ can assume $n_j$ values.

| $X\backslash Y$ | 1 | 2 | 3 |
|---|---|---|---|
| 1 | 0.15 | 0.08 | 0.07 |
| 2 | 0.01 | 0.2 | 0.03 |
| 3 | 0.28 | 0.17 | 0.09 |

Table 3.1: Joint probability table for $X$ and $Y$.

$$P(X = x) = \sum_{j_1=1}^{n_1} \ldots \sum_{j_m=1}^{n_m} P(X = x, Z_1 = z_{j_1}, \ldots, Z_m = z_{j_m}) \tag{3.22}$$

For exercise purposes, it often helps to draw a joint probability table and do marginalization from there.

**Exercise 3.14** *Find the marginal distributions $P_X$ and $P_Y$ in Table 3.1.*

We have already seen how the joint probability of random variables links back the the probability space that underlies them. This link makes it easy to import certain concepts that we have gotten to know in previous chapters. In particular, we can define **conditional probability distributions**.

**Definition 3.15 (Conditional probability distribution)** *Let $X, Y$ be random variables with joint distribution $P_{XY}$. Let $y$ be such that $P(Y = y) > 0$. The probability of $X = x$ conditioned on $Y = y$ is given by*

$$P(X = x|Y = y) := \frac{P(X = x, Y = y)}{P(Y = y)}.$$

*The conditional distribution of $X$ given $Y = y$ is denoted by $P_{X|Y=y}$.*

**Exercise 3.16** *Compute the conditional probability distributions $P_{X|Y=2}$ and $P_{Y|X=1}$ from Table 3.1.*

Likewise, the concept of independence carries over to distributions.

**Definition 3.17 (Independence of random variables)** *Two random variables $X, Y$ are independent (denoted by $X \perp Y$) if $P_{XY} = P_X P_Y$, i.e. $\forall x \in \operatorname{supp}(X), \forall y \in \operatorname{supp}(Y) : P(X = x, Y = y) = P(X = x)P(Y = y)$.*

As with events, independence is equivalent to stating that $P_{X|Y} = P_X$ (and to $P_{Y|X} = P_Y$). Moreover, independence makes it much easier to calculate the expectation and variance of functions of jointly distributed random variables. For independent $X$ and $Y$, we have

$$\begin{aligned}
\mathbb{E}[XY] &= \sum_{x\in\text{supp}(X)} \sum_{y\in\text{supp}(Y)} P(X=x, Y=y)xy && (3.23)\\
&= \sum_{x\in\text{supp}(X)} \sum_{y\in\text{supp}(Y)} P(X=x)P(Y=y)xy && (3.24)\\
&= \sum_{x\in\text{supp}(X)} P(X=x)x \sum_{y\in\text{supp}(Y)} P(Y=y)y && (3.25)\\
&= \mathbb{E}[X]\mathbb{E}[Y] && (3.26)
\end{aligned}$$

Similarly, it does not really make sense to talk about the variance of two random variables (at least not as one single value). However, we can again compute the variance of functions. For addition, independence again makes our lives much easier.

**Exercise 3.18** *Show that for independent RVs $X$ and $Y$, we have that* $\text{var}(X+Y) = \text{var}(X) + \text{var}(Y)$. *Give an example of dependent $X$ and $Y$ with* $\text{var}(X+Y) \neq \text{var}(X) + \text{var}(Y)$.

While the variance of two jointly distributed variables is not defined, there is the concept of **covariance**. The variance measures the spread of one RV, the covariance measures to what extend two variables spread together. In other words, to what extend two variables change together systematically.

**Definition 3.19 (Covariance)** *The covariance of two RVs $X, Y$ with joint distribution $P_{XY}$ is defined by*

$$cov(X,Y) := \mathbb{E}\left[(X - \mathbb{E}[X])\,(Y - E[Y])\right]$$

**Exercise 3.20** *Define any two random variables with joint distribution $P_{XY}$ such that $cov(X,Y) < 0$.*

Notice that covariance is symmetric. Let us for a moment look at it as a function of $X$ only. Then, for every value $y \in \operatorname{supp} Y$, the quantity $(y - \mathbb{E}[Y]) = c_y \in \mathbb{R}$ serves as a coefficient which scales $(X - E[X])$ and that thus determines how much the covariance changes as we change $P_X$. Under this view, the covariance is be a linear function of $X$. The precise meaning of saying that the covariance measures the systematic joint change of $X$ and $Y$ is thus that it measures their linear dependence on each other.

Another interesting question is to what extend two variables influence each other relatively, i.e. how much the outcome of one determines the outcome of the other. The general concept behind this question is called **correlation**. Correlation is always a measure of dependence between two RVs.

Recall that the definition of independence is binary – either two variables are independent or they are not. Correlation allows us to make more fine-grained relationships between RVs. There are different measures of correlation. We present the quasi-standard one here.

**Definition 3.21 (Pearson Correlation)** *The Pearson correlation coefficient between to RVs $X$ and $Y$ with finite non-zero variance and joint distribution $P_{XY}$ is given as*

$$\rho_{XY} = \frac{cov(X,Y)}{\sigma(X)\sigma(Y)}$$

*where $\sigma(X) = \sqrt{\text{var}(X)}$.*

The correlation coefficient $\rho$ measure the dependence between variables through their (co)variances. It does so by normalizing each of the two RVs to having unit variance. The Pearson correlation is then simply the covariance of the normalized variables. Notice that because the covariance can take on both positive and negative values, the Pearson correlation lies in the interval $[-1, 1]$. The interpretation of $\rho_{XY}$ is thus that it measure the relative linear influence (dependence) of the variables on one another. This is different from the covariance which measures the absolute linear dependence that the variables have on each other. Notice that covariance and correlation are closely related, so much in fact that one sometimes sees the following definition of covariance.

$$cov(X,Y) = \rho_{XY}\sigma(X)\sigma(Y) \tag{3.27}$$

As with expectation and variance, independence of two variables also has consequences for their correlation and covariance.

**Exercise 3.22** *Assume two RVs $X$ and $Y$. Show that if $X \perp Y$ we have $cov(X,Y) = 0$ and $\rho_{XY} = 0$.*

## 3.4 Some Important Distributions

We will finish this chapter by introducing some extremely useful discrete distributions. They are very often used in computer science to model the probability of bit strings and in linguistics and natural language processing to model the probability of sentences.

To get us started, let us consider coin tosses. When you toss a fair coin, the probability that it lands on heads is 0.5 and so is the probability that it lands on tails. Let 1 stand for heads and 0 for tails in a random variable $X$ modelling coin tosses. We can formalize this distribution as

$$P(X = x) = 0.5^x \times 0.5^{1-x} = 0.5 \text{ for } x \in \{0, 1\} \ .$$

Notice though that not all coins are fair and that in general we want to allow for probabilities that are not equal. We will therefore introduce a parameter $\theta$ that regulates the probability that we observe heads. In the above equation, we set $\theta = 0.5$. What happens if we set $\theta = 0.3$?

$$P(X = x) = 0.3^x \times 0.7^{1-x} = \begin{cases} 0.3 & \text{if } x = 1\,, \\ 0.7 & \text{if } x = 0\,. \end{cases} \tag{3.28}$$

Where did we get the 0.7 from? Well, we know that the coin has to land on either heads or tails. Thus, if the probability to land on heads is 0.3 the probability to land on tails has to be 0.7. Moreover, we chose 1 as a stand-in for landing on heads. As we would expect, $X = 1$ will return the 0.3 probability and $X = 0$ will return the probability of 0.7.

This leads to a general formulation where we do not specify the parameter $\theta$ but leave it to be filled in. The resulting distribution, known as **Bernoulli distribution** (with parameter $\theta$), is shown in Equation (3.29).

$$P(X = x) = \theta^x \times (1-\theta)^{1-x} = \begin{cases} \theta & \text{if } x = 1\,, \\ 1-\theta & \text{if } x = 0\,. \end{cases} \tag{3.29}$$

The Bernoulli is defined for one coin flip, or more generally for the drawing of a coloured ball from a (very large) urn containing balls of exactly two colours (in proportion $\theta$ and $1 - \theta$). What if we draw balls repeatedly with replacement? We will get a sequence of coloured balls. Say we draw $n$ balls and repeat this procedure five times. Chances are that the five sequences will look rather different. Thus, we can define a probability distribution over sequences of coloured balls of length $n$. This procedure can be described as a simple generalization of the Bernoulli. Whereas in the Bernoulli we made one draw we make $n$ draws. This yields a sequence $x$ in which each position $x_i, 1 \leq i \leq n$ is either 0 or 1. We speak of **repeated Bernoulli trials** in this case.

$$P(X = x) = \prod_{i=1}^{n} \theta^{x_i} \times (1-\theta)^{1-x_i} = \theta^{\sum_i x_i} \times (1-\theta)^{n-\sum_i x_i} \tag{3.30}$$

The adjustment is rather small. We basically only introduce an extra parameter, namely the number of draws $n$. However, there are two conditions for this distribution that we have not mentioned yet. First and foremost, the repeated Bernoulli draws are assumed to be independent. That is, for each draw in the sequence it should not matter which colours you have drawn so far and which ones you are still going to draw (as you are drawing with replacement). More formally, if we encode each draw in the sequence as a random variable, we postulate that these random variables are independent of each other.

The second point is that we cannot assign a probability to any sequence that contains more balls of one colour than there are balls in total. This is to say that we require that $0 \leq \sum_{i=1}^{n} x_i \leq n$ which is a reasonable restriction.

It is also worth mentioning that in general the two values that the distributions in (3.29) and (3.30) range over are generally referred to as success and failure where the success is usually encoded as 1 and the failure as 0.

**Exercise 3.23** *Use the distribution in Equation* (3.30) *with* $n = 10$ *and* $\theta = 0.8$ *to determine the probability of the sequence (0,0,1,1,0,1,1,1,0,1).*

Another interesting observation is that, since the value at each position in the sequence is independent of all others, all sequences with the same number of successes and failures will have the same probability. At this point it is natural to ask for the probability to get *any* sequence with that amount of successes and failures. Say we are dealing with sequences of length $n$ and wonder about the probability of obtaining a sequence with $0 \leq k \leq n$ successes. Then we simply need to sum up the probabilities of all sequences that contain $k$ successes. But how many such sequences are there? In Chapter 1, we talked about how to choose a subset of $k$ elements out of $n$. This is exactly the problem we are facing here. We want to know how many ways there are to choose $k$ out of $n$ positions that we interpret as successes. This counting is done by the binomial co-efficient $\binom{n}{k}$.

We can generalize the distribution from Equation (3.30) to a distribution that gives the probability of obtaining any sequence with $k$ successes. This distribution is known as the **binomial distribution** (with parameters $n$ and $\theta$).

$$P(X = k) = \binom{n}{k} \theta^k (1 - \theta)^{n-k} \tag{3.31}$$

The binomial is of crucial importance in many fields. For example in computer science, it is used to compute the probability of bit strings. Other applications include the assessment of failure rates. Say you run a company and a customer asks you to supply $k$ items within a week. The capacity of your company allows you to produce at most $n > k$ items during that week. At the same time you know that each item that you produce has a probability of being faulty. Obviously, you cannot sell faulty items to your customer. The binomial distribution allows you to compute the probability that you will be able to meet the customer's demand. Based on this calculation, you can evaluate whether or not it is reasonable to accept the customer's order.

Bernoulli and binomial distributions are of course limited to RVs with only two outcomes. We are now going to generalise them for RVs with any finite number of outcomes. Let us call the number of outcomes $k \in \mathbb{R}$. What we are essentially doing then is flipping a $k$-sided coin. As with a two-sided coin, the coin needs to land on one of its sides, however, it may also be biased. We thus have one parameter $\theta_j$ for each side of the coin with the restriction that $\sum_{j=1}^{k} = 1$. Notice that because of this restriction we actually only have $k-1$ parameter since $\theta_k = 1 - \sum_{j=1}^{k-1} \theta_j$. For notational convenience we will work with $k$ parameters, tough. Finally, let us introduce the indicator function

$$\mathbb{I}_x(j) = \begin{cases} 1 & \text{if } x = j \\ 0 & \text{otherwise} \end{cases} . \tag{3.32}$$

We can now define the generalisation of the Bernoulli which is known as the **categorical** distribution.

$$P(X = x) = \prod_{j=1}^{k} \theta_j^{\mathbb{I}_x(j)} \tag{3.33}$$

Just as with the Bernoulli distribution, we can also have **repeated categorical trials**. Recall that repeated trials are independent (i.e. we draw outcomes with replacement). The probability of outcomes $x_1^n$ under repeated categorical trial is

$$P(X_1^n = x_1^n) = \prod_{i=1}^{n} \prod_{j=1}^{k} \theta_j^{\mathbb{I}_{x_i}(j)} = \prod_{j=1}^{k} \theta_j^{\sum_{i=1}^{n} \mathbb{I}_{x_i}(j)} . \tag{3.34}$$

Notice that repeated categorical trials assign probabilities to sequences of outcomes. We can again ask the question what the probability of obtaining *any* sequence with a specified number of each outcome is. This brings us to the next distribution that we get to know today: the **multinomial distribution**. It is basically a generalization of the binomial. Let us assume that outcome $j$ occurs $c_j$ times in a sequence of length $n$ where $1 \leq i \leq n$ and $\sum\limits_{i=1}^{m} c_i = n$. Summing over all the sequences that have this property means finding all the ways to draw $c_j$ observations (for each outcome $j$) from a total of $n$ observations. This is accomplished by calculating the multinomial coefficient. Therefore, the multinomial distribution with parameters $n$ and $\theta_1, \ldots, \theta_n$ is given as

$$P(X_1^n = x_1^n) = \frac{n!}{\prod\limits_{j=1}^{k} c_j!} \prod_{j=1}^{k} \theta_j^{\sum_{i=1}^{n} \mathbb{I}_{x_i}(j)} \tag{3.35}$$

It is easy to see that the binomial is in fact just the special case $m = 2$ of the multinomial. Because of its general importance it is usually considered a separate distribution though.

Let us finish this section by introducing some useful notation. When a RV is distributed according to some distribution, one often uses the tilde($\sim$) to express this fact. If, for example, we have a random variable $X$ that is distributed according to a binomial with $n = 100$ and $\theta = 0.5$, many authors will write

$$X \sim binom(100, 0.5)$$

Now that we know what it means for a random variable to be distributed according to some distribution, we can also clarify a question that was brought up in the beginning. What does sampling *uniformly at random* mean? It just means that we are sampling from a distribution that is the uniform distribution (all values in the support have the same probability). The *random* comes from the fact that we are sampling the values of a random variable. Just saying that some quantity is sampled at random is not enough. You should always add which distribution underlies that randomness!

## 3.5 Other Interesting Distributions

Another interesting distribution that is well worth looking at is the negative binomial distribution. Suppose we do repeated independent Bernoulli trials and we wonder how many trials it will take until we have observed $k > 0$ successes. To answer this question, we would like to assign a probability to each integer $t \geq k$ which can be interpreted as the probability that we will take $t$ trials until we have obtained the desired number of successes. Notice that for each $t$, we can infer the number of failures as $f = t - k$.

To approach this problem, let us start out from the simplest case where we are only waiting for one success. In that case, our sequence of trials ends in a success, which is also the only success in the sequence. Thus the sequence contains $f = t - 1$ failures. The success probability of a Bernoulli trial is $\theta$, as usual. Then the associated probability distribution for $T$ with parameters $\theta$ and $k = 1$ is

$$P(T = t) = \theta^1 (1 - \theta)^{t-1} \tag{3.36}$$

Equation (3.36) is known as the **geometric distribution**. It models the discrete waiting time until an event occurs. Somewhat confusingly, there are two versions of the geometric distribution. The one given in (3.36) does not allow for the waiting time to be 0. It will always be at least 1, even if when our first draw is already a success. Sometimes one does want to allow for 0 waiting time, however. In that case, one uses a geometric distribution that looks as follows:

$$P(T = t) = \theta^k (1 - \theta)^t \ . \tag{3.37}$$

While it is safe to work with only one of these (after all we can transform them by simply adding or subtracting 1 to their outcomes), be aware of the difference when working with software, for example, where only one of the two versions will be implemented.

Notice that if $k = 1$ there is only one sequence of size $t$ that ends in a success. If we let $k > 1$, there are more sequences of length $y$ that end in a success and contain $k$ successes in total. The probability for any such sequence can easily be calculated by generalising Equation (3.36).

$$P(T = t) = \theta^k (1 - \theta)^{t-k} \tag{3.38}$$

As with the Binomial, we now have to add up the probabilities of all sequences of length $t$ that contain exactly $k$ successes *and end in a success.* The last condition is what separates the negative Binomial from the Binomial distribution. We first observe that the position of the last success is fixed. This means we are left with $k - 1$ which we can assign to different positions. In total there are $t-1$ positions that we can assign. Thus we have to choose $k - 1$ out of $t - 1$ position over which to distribute the remaining $k - 1$ successes. Thus, we conclude that there are $\binom{t-1}{k-1}$ sequences of length $t$ that contain $k$ successes, one of which occurs in the last position of the sequence. This is allows us to define the negative Binomial distribution with parameters $\theta$ and $k$ as

$$P(T = t) = \binom{t-1}{k-1} \theta^k (1 - \theta)^{t-k} \tag{3.39}$$

where $t \in \mathbb{N}, t > k$.

Many authors use the notation $X \sim nbinom(\theta, k)$ to state that the RV $X$ is distributed according to a negative Binomial distribution.

# Chapter 4

# Bayes' rule and its applications

## 4.1 The chain rule

This chapter is going to focus on how to re-write joint and conditional probabilities. When we turn to statistics later on, it will turn out that it is often hard to define a joint distribution over many variables. Likewise, it can be hard to calculate the probability distribution of a RV $X$ conditioned on a RV $Y$ but it may be much easier to find the distribution of $Y$ conditioned on $X$. In this chapter we are essentially trying to find simpler expressions for distributions that may be hard to compute.

The first general method for simplifying a joint distribution is known as the **chain rule**. For completeness' sake, we are going to formulate the chain rule first for events and then for random variables.

**Theorem 4.1** ***(Chain rule)*** *The joint probability of events $E_1, \ldots, E_n$ can be factorised as*

$$\mathbb{P}(E_1, \ldots, E_n) = \mathbb{P}(E_1) \times \mathbb{P}(E_2|E_1) \times \ldots \times \mathbb{P}(E_n|E_1, \ldots, E_{n-1})$$

Recall from Definition 2.6 the notation $\mathbb{P}(E_1, E_2) = \mathbb{P}(E_1 \cap E_2)$ for denoting the probability that both events $E_1$ and $E_2$ occur. Also remember that we use the abbreviation $E_1^n := E_1, \ldots, E_n$; so for the case of events, we have $\mathbb{P}(E_1^n) = \mathbb{P}(\bigcap_{i=1}^n E_i)$. There are a couple of things to note about the chain rule: First of all, the numbering of the events is arbitrary. That means that it does not matter in which order we decompose the joint probability. We could just as well start with any $E_i$ for $1 \leq i \leq n$. Second we used the word *factorise*. This simply means that we decompose any expression (in this case a joint probability) into a product. Products are nice in that we can arrange them in any order that we like (i.e. they commute). Moreover, products make a lot of calculations easier, as we will see later.

Let us go ahead and actually prove the chain rule.

**Proof of Theorem 4.1** We are going to do so inductively and choose $\mathbb{P}(E_1, E_2)$ as our base case. Then we simply employ the definition of conditional probability to get

$$\mathbb{P}(E_1, E_2) = \mathbb{P}(E_1) \times \frac{\mathbb{P}(E_1, E_2)}{\mathbb{P}(E_1)} = \mathbb{P}(E_1) \times \mathbb{P}(E_2|E_1) \tag{4.1}$$

Let us assume that the chain rule holds for events $E_1, \ldots, E_{n-1}$. We will abbreviate them as $E_1^{n-1}$. Then we get

$$\mathbb{P}(E_1^{n-1}, E_n) = \mathbb{P}(E_1^{n-1}) \times \frac{\mathbb{P}(E_1^{n-1}, E_n)}{\mathbb{P}(E_1^{n-1})} = \mathbb{P}(E_1^{n-1}) \times \mathbb{P}(E_n|E_1^{n-1}) \tag{4.2}$$

Since $\mathbb{P}(E_1^{n-1})$ factorises according to the chain rule by our induction hypothesis, we have completed the proof. □

The chain rule can make our lives even simpler if we have independent events. Assume we want to compute the joint probability of 3 events $E_1, E_2, E_3$ and we also know that $E_1 \perp E_2$. In this case our factorisation becomes (4.3) where the first equality follows from the chain rule and the second equality follows from independence between $E_1$ and $E_2$.

$$\begin{aligned} \mathbb{P}(E_1, E_2, E_3) &= \mathbb{P}(E_1) \times \mathbb{P}(E_2|E_1) \times \mathbb{P}(E_3|E_1, E_2) \\ &= \mathbb{P}(E_1) \times \mathbb{P}(E_2) \times \mathbb{P}(E_3|E_1, E_2) \end{aligned} \tag{4.3}$$

We can now state the chain rule for random variables. There are two ways you can go about proving it. Either you calculate the probability of a specific setting of the variables or you just do the proof based on the distributions of the RVs. So in the first case you would have to prove that

$$\begin{aligned} \forall x_1, \ldots, x_n : &P(X_1 = x_1, \ldots, X_n = x_n) \\ &= P(X_1 = x_1) \times \ldots \times P(X_n = x_n|X_1 = x_1, \ldots, X_{n-1} = x_{n-1}) \end{aligned}$$

whereas in the second case you would simply prove that

$$P_{X_1^n} = \sum_{i=1}^{n} P_{X_i|X_1^{i-1}}$$

Incidentally, we also introduce a very short notation for the chain rule above. Note that it is not quite correct, since if $i = 1$ we would be conditioning on $X_0$. That is not to bad however, since we can always define ourselves a constant variable $X_0$ that does not affect the distribution. Moreover, this notation is really just meant to be convenient, so you should just accept it as is when you encounter it in papers.

**Exercise 4.2** *Prove the chain rule for random variables. The proof is totally analogous to the one give for events.*

**Exercise 4.3** *Let $X_0$ be a constant RV, i.e. there exists $c \in \mathbb{R}$ such that $P(X_0 = c) = 1$. Prove that $X_0$ is independent of any set of other random variables $X_1, \ldots, X_n$.*

## 4.2 Bayes' rule

In this section we are going to prove **Bayes' rule**. The rule follows directly from the chain rule. The proof is really simple and thus of no great interest in and by itself. The consequences of Bayes' rule are huge however. It will basically allow us to invert a conditional probability distribution. You may rightfully ask: what's the deal? Well, as we said in the beginning, it may be hard to compute a conditional distribution in one direction but much easier to compute it in the other direction. On top of that, Bayes' rule opens up a whole range of new possibilities. We will discuss those as we proceed in this chapter.

**Theorem 4.4** ***(Bayes' rule)*** *The probability distribution of a random variable $X$ given a random variable $Y$ can be computed as*

$$P_{X|Y} = \frac{P_{Y|X} P_X}{P_Y}$$

And here comes the proof:

$$P_{X|Y} = \frac{P_{XY}}{P_Y} = \frac{P_{Y|X} P_X}{P_Y} . \qquad \square \tag{4.4}$$

That was the proof! Considering how simple it was, it will be surprising to see what kind of benefits we can get out of Bayes' rule. To get us started, let us introduce some terminology. In particular, each of the terms in Bayes' rule has a specific name. You should really learn these names by heart as they crop up all over the place.

$$\textit{posterior} = \frac{\textit{likelihood} \times \textit{prior}}{\textit{marginal likelihood}}$$

The posterior is what we get after we have completed the computation. However, its name is related to the prior. The prior is just the probability that we would place on $P(X = x)$ *a priori*. Therefore $P_X$ is also known as the prior distribution. When we divide the product of likelihood and prior by the marginal likelihood we get a new distribution over $X$ that is conditioned on $Y$. This is the distribution that we place on $X$ *a posteriori*, i.e. after having taken into account information about $X$ that we may get from knowing the value of $Y$. The marginal likelihood of $Y$ is simply needed to normalize the expression to a probability distribution (i.e. to make sure that it sums to one). Why is it called marginal likelihood? The reason for this is how you can compute it. Recall that when we are given a joint distribution $P_{XY}$, we can obtain the distribution $P_Y$ by simply marginalizing over $X$.

$$P(Y = y) = \sum_{x \in \text{supp}(X)} P(X = x, Y = y) \tag{4.5}$$

In addition to that, the chain rule allows us to factorise the joint probability. Thus we get

$$P(Y = y) = \sum_{x \in \text{supp}(X)} P(Y = y|X = x) \times P(X = x) \tag{4.6}$$

If you think that this looks an awful lot like the enumerator of Bayes' rule then you are exactly on the right track. Essentially, we are just summing over all possible denominators (with respect to $X$). Let us make this more concrete with an example. Assume that we are given two coins. One of them is fair, meaning that it is equally probable to come up heads or tails. The other coin is biased towards tails and we happen to know that its probability to come up heads is only 0.3. Which coin is flipped is captured by a random variable $X$ that takes on the value 0 if the fair coin is used and the value 1 if the biased coin is used. We have no idea which coin is going to be tossed, it could be either one. Therefore we set our prior to $P(X = 0) = P(X = 1) = 0.5$.

We flip the chosen coin 10 times and obtain 8 heads. The number of heads obtained during the 10 tosses is going to be encoded by $Y$. Since all tosses are independent of each other, $Y$ will follow a binomial distribution. For each of the two coins we also know the parameter of the binomial distribution. For the fair coin it is $\theta = 0.5$ and for the biased coin it is $\theta = 0.3$. Let us compute each of the enumerators separately.

$$P(Y = 8|X = 0) \times P(X = 0) = \binom{10}{8} 0.5^8 (1 - 0.5)^2 \times 0.5 = 0.02195 \tag{4.7}$$

$$P(Y = 8|X = 1) \times P(X = 1) = \binom{10}{8} 0.3^8 (1 - 0.3)^2 \times 0.5 = 0.0007 \tag{4.8}$$

Remember that $Y \sim \mathit{binom}(10, \theta)$ and that $\theta = 0.5$ if $X = 0$ and $\theta = 0.3$ if $X = 1$.

All that is left do is to compute the marginal likelihood of $Y$. Luckily for us, $X$ only assumes two values, so we only need to add up (4.7) and (4.8).

$$\begin{aligned} P(Y = 8) = & P(Y = 8|X = 0) \times P(X = 0) \\ & + P(Y = 8|X = 1) \times P(X = 1) = 0.02265 \end{aligned} \tag{4.9}$$

And finally we can apply Bayes' rule to compute the posterior probabilities of $X$.

$$P(X=0|Y=8) = \frac{P(Y=8|X=0)\times P(X=0)}{P(Y=8)} \tag{4.10}$$
$$= \frac{0.2195}{0.02265} = 0.969$$
$$P(X=1|Y=8) = \frac{P(Y=8|X=1)\times P(X=1)}{P(Y=8)} \tag{4.11}$$
$$= \frac{0.0005}{0.02265} = 0.031$$
$$\tag{4.12}$$

There is a probability of 0.969 that the fair coin has been tossed when a sequence with eight heads is generated and only a probability of 0.031 that the biased coin was tossed. Obviously, the probability of the fair coin is much higher. But how much higher? We can take the ratio of the two probabilities. This gives us $^{0.969}/_{0.031} \approx 31$. We can conclude that the fair coin is 31 times more likely to have generated the sequence with 8 heads than the biased coin. But wait a second, can we maybe find this ratio somewhere else? It turns out that the ratio of the likelihoods is the same! That is $^{0.0439}/_{0.0014} \approx 31$.

We started out by assuming that both coins were equally likely to be used. However, we then observed a sequence of 10 tosses, 8 of which were heads and that made it 31 times more likely that the fair coin was used. What if the priors had not been equal? Actually, there is a more general story: While calculating the actual probabilities involves a lot of number crunching, just telling whether or not an observation will make one or the other event more likely is not too hard. [For the rest of this chapter, we assume that we only condition on events with non-zero probabilities such as $P(Y=y)>0$ so that we are never dividing by 0].

$$\frac{P(X=x_1|Y=y)}{P(X=x_2|Y=y)} = \frac{\dfrac{P(Y=y|X=x_1)P(X=x_1)}{P(Y=y)}}{\dfrac{P(Y=y|X=x_2)P(X=x_2)}{P(Y=y)}}$$

$$= \frac{P(Y=y|X=x_1)P(X=x_1)}{P(Y=y|X=x_2)P(X=x_2)}$$

From the above equalities, we see that the ratio of the posterior probabilities is determined by the ratio of the likelihood times the prior. In our coin example, the priors were the same so it was only the likelihood that mattered. If the ratio of any of the above terms is greater than 1, the posterior will change in favour of $X=x_1$. If the ratio is smaller than 1 the posterior changes in favour of $X = x_2$. If the ratio is exactly 1, the posterior stays unchanged.

Notice that in general, although our observations may shift the posterior in favour of $X = x_2$, say, this shift does not necessarily imply that $P(X = x_2|Y = y)$ will be greater than $P(X = x_1|Y = y)$. The condition that $P(X = x_2|Y = y)$ is bigger than $P(X = x_1|Y = y)$ can be rewritten as follows

$$\begin{aligned}
P(X = x_1|Y = y) &< P(X = x_2|Y = y) & \Leftrightarrow \\
\frac{P(Y = y|X = x_1)P(X = x_1)}{P(Y = y)} &< \frac{P(Y = y|X = x_2)P(X = x_2)}{P(Y = y)} & \Leftrightarrow \\
P(Y = y|X = x_1)P(X = x_1) &< P(Y = y|X = x_2)P(X = x_2) & \Leftrightarrow \\
\frac{P(Y = y|X = x_1)}{P(Y = y|X = x_2)} &< \frac{P(X = x_2)}{P(X = x_1)}
\end{aligned}$$

The last line is of particular interest as it elucidates the relationship between the prior and the likelihood. Only if the likelihood ratio for $X = x_1$ over $X = x_2$ is smaller than the reversed prior ratio will the posterior probability of $X = x_2$ be greater than that of $X = x_1$. This means that if we have strongly asymmetric priors (like $P(X = x_1) = 0.9$ and $P(X = x_2) = 0.1$), the likelihood needs to discriminate very well between the two cases in order to tip the scale in favour of $X = x_2$. In that sense the prior and the likelihood can be seen as battling forces whose equilibrium gives us the posterior.

But enough theory about Bayes' rule, it is about time you apply it! To that end, we present you an exercise that is, in some variation, contained in virtually every textbook on probability theory, statistics or machine learning. Have fun with it!

**Exercise 4.5** *A random person walks into the doctor's office to be tested for a particular disease. The disease can be fatal if not treated. However, successful treatment is possible if the disease is discovered early enough. It is commonly known that the disease occurs in 1 out of 1000 people of the country's population. The doctor will administer a test that with a probability of 99% returns a positive results if the patient does indeed have the disease. At the same time, the test also returns a positive result in 5% of the cases where the patient does not have the disease. After the test has been administered to the patient in question, it returns a positive result. What is the probability that the patient is infected with the disease?*
*Proceed as follows:*

1. *Write down a guess for what you think the probability might be (do not consider any math at this point).*

2. *Calculate that probability.*
3. *Check whether there is a considerable difference between your initial guess and the calculated probability. Go on to examine how the different factors have influenced the probability of the patient having the disease.*

Let us finish up this section with some more notation. In many applications of Bayes' rule we only want to know which outcome is the most likely, without worrying too much about the actual probabilities. Likewise, there is a range of situations where we just want to assign a score to outcomes and do not demand this score to be a probability. Throughout this chapter, we have repeatedly encountered the following phenomenon: In order to rank the values of an RV according to their probabilities, we do not necessarily need to compute the marginal likelihood since it cancels in all these comparisons anyway. Therefore, you will often see authors stating that

$$P(X = x|Y = y) \propto P(Y = y|X = x)P(X = x) \tag{4.13}$$

This equation reads as "the posterior is proportional to the product of the likelihood and the prior". In general, if we have two quantities $a$ and $b$, then by $a \propto b$ we mean that there is some constant $C \in \mathbb{R} \setminus \{0\}$ such that $a = Cb$. Notice that the probability distribution is a function and hence we require $C$ to be the same across the domain of that function (that is $C$ should be the same for all values of $X$).

**Exercise 4.6** *What is the value of $C$ in Equation (4.13)?*

## 4.3 Naïve Bayes

In this section, we introduce a rather crude application of Bayes's rule which is surprisingly successful nonetheless. Assume that instead of one random variable we are observing a sequence of random variables. Thus our problem is the following:

$$P(Y = y|X_1^n = x_1^n) \propto P(X_1^n = x_1^n|Y = y) \times P(Y = y) \tag{4.14}$$

By the chain rule we can decompose the right-hand side into

$$\begin{aligned} P(Y = y|X_1^n = x_1^n) \propto & P(X_1 = x_1|Y = y) \times \ldots \\ & \times P(X_n = x_n|Y = y, X_1^{n-1} = x_1^{n-1}) \times P(Y = y) \end{aligned}$$

We are now going to introduce the aforementioned crudeness into the model by assuming that all $X_1, \ldots, X_n$ are conditionally independent given $Y$. Notice that this is just an assumption that we are making without justification. In fact, it is very likely wrong. However, it makes our live much easier because we only have to deal with very simple terms of the form $P(X_i = x_i|Y = y)$. Because of the crudeness of our assumptions, this probabilistic model is known as **naïve Bayes** (sometimes also stupid Bayes).

**Definition 4.7** *A naïve Bayes model is a probabilistic model that assumes*

$$P_{Y|X_1^n} \propto P_Y P_{X_1|Y} P_{X_2|Y} \cdots P_{X_n|Y}$$

Once we know all the component distributions $P_{X_i|Y}$, calculating the result is pretty straightforward.

In order to illustrate how naïve Bayes works we are going to employ one of its showcase applications where it indeed had a lot of success in real life. The application we are talking about is text classification. The task is the following: you are given some documents and for each of the documents you have to assign a label signifying its class. What you consider a class depends on your actual application setting, but usually classes are broad categories, such as legal texts, medical texts etc. If you manage to succeed at this task, you can accomplish a lot of things automatically that required humans before. For example, you could tag online news with their relevant categories and people who are interested in a particular category will then have an easier time finding the news related to that category. Crucially, since you will write a computer program that does the classification for you, you will not need to read any of the texts yourself. This automation will obviously allow you to classify huge quantities of text in a very short amount of time.

**Exercise 4.8** *A collection of text (or any other kind of data for that matter) is often called a* ***corpus****. Here we are going to use a toy corpus. The corpus just consists of two sentences and we assume that each sentence constitutes a document. The categories that you can label the documents with are finance (0), medicine (1) or law (2). You can find the corpus (the pmfs of the distributions) below. For simplicity, we are not going to distinguish between lower and upper case words (this is actually common practice). For better readability, we are also using the actual words instead of their numerical encodings as values for the random variables. Just remember that those words could also be represented as real random variables. To shorten notation, we will use pmfs. If the probability of a word given a category is not specified, take it to be 0.*

*Your task is to classify these two documents correctly using a Naïve Bayes Model that conditions each word's probability on the document class. Please also report the posterior probability for the correct label.*

**The corpus:**

- a fact has been revealed
- the doctor's judgement has not been reliable

**The document category pmfs:**

- $p(0) = 0.3$
- $p(1) = 0.2$
- $p(2) = 0.5$

**The lexical distribution for document category finance (0):**

$$p(a|0) = 0.19 \;\; p(\mathit{fact}|0) = 0.14 \;\; p(\mathit{has}|0) = 0.13 \;\; p(\mathit{been}|0) = 0.12$$
$$p(\mathit{revealed}|0) = 0.04 \;\; p(\mathit{the}|0) = 0.21 \;\; p(\mathit{doctor's}|0) = 0.03$$
$$p(\mathit{judgement}|0) = 0 \;\; p(\mathit{not}|0) = 0.11 \;\; p(\mathit{reliable}|0) = 0.03$$

**The lexical distribution for document category medicine (1):**

$$p(a|1) = 0.02 \;\; p(\mathit{fact}|1) = 0.08 \;\; p(\mathit{has}|1) = 0.13 \;\; p(\mathit{been}|1) = 0.13$$
$$p(\mathit{revealed}|1) = 0.01 \;\; p(\mathit{the}|1) = 0.18 \;\; p(\mathit{doctor's}|1) = 0.06$$
$$p(\mathit{judgement}|1) = 0.14 \;\; p(\mathit{not}|1) = 0.20 \;\; p(\mathit{reliable}|1) = 0.05$$

**The lexical distribution for document category law (2):**

$$p(a|2) = 0.18 \;\; p(\mathit{fact}|2) = 0.03 \;\; p(\mathit{has}|2) = 0.05 \;\; p(\mathit{been}|2) = 0.13$$
$$p(\mathit{revealed}|2) = 0.10 \;\; p(\mathit{the}|2) = 0.14 \;\; p(\mathit{doctor's}|2) = 0.06$$
$$p(\mathit{judgement}|2) = 0.07 \;\; p(\mathit{not}|2) = 0.08 \;\; p(\mathit{reliable}|2) = 0.16$$

## Further Reading

Here, we have only scratched the surface of what Bayes' rule allows us to do. To get a wider outlook on what else is possible, you can consult Kevin Murphy's webpage.

# Chapter 5

# Statistics: what it is and why it works

## 5.1 Motivation

By now, we have learned a whole lot about probability theory. In the previous chapter we have seen how to compute the distribution of a RV given another RV. Moreover, we know how to factor joint distributions and simplify them by making independence assumptions. In principle, this puts us in a good position to start formulating our own probabilistic models. However, our models will be pretty useless if we do not know their parameters. And as it so happens, we virtually never know them in real life. So what we are going to talk about next is how to **estimate** these parameters from data that we observe. The tools we are going to use for estimation come from statistics.

Statistics is a relatively broad term. There are many ways of doing it and chances are that different people from different fields mean different things when they use the term *statistics.* This is mostly so because the goals that people want to achieve using statistics are different. The underlying mechanics do in fact not differ that much. In this course, we are going to focus on the basics of statistics that you need to know no matter what your goals are. However, allow us to give you a quick birds-eye view on statistics.

There are two main goals you can have using statistics (this is grossly oversimplified, but hey, we said it was the birds-eye view). On the one hand you can do **descriptive statistics** which means that you are gathering information about a phenomenon that you are interested in and report that information. For example, you might be interested in how many faculty members at your university are alcoholics. What you do is you go to each faculty member, check whether they are an alcoholic and report the total number of alcoholics at your institute. Crucially, you are not going to draw any conclusions (such as that people working in the humanities are more likely to be alcoholics than those working at the science faculty).

Another, somewhat milder example of descriptive statistics are housing advertisements. If you are looking for a flat, you will usually find descriptions of the offered flats in terms of square metres, storey, the presence of a balcony, etc. All of these descriptions can be seen as descriptive statistics. Again, when reviewing these ads, your goal will not be to make a statement like "flats with a balcony are more habitable than flats without one". This may be your own preconception, but it is nothing that you would be trying to get out of your data.

The second big part of statistics is **inferential statistics**. Here you are actually interested in drawing conclusions (inferences). So if you do an alcoholism survey amongst faculty at your university, you would like to find some way of determining the relationship between area of research, say, and the chance that someone is an alcoholic. The rest of the course will mostly be about inferential statistics. In particular, our main question will be the following: given that we observe some data and we know (or assume) that the data is distributed according to some distribution (e.g. a multinomial) what are the parameters of that distribution? Hence, we will try to infer the parameters.

Within inferential statistics, there is a further distinction one can make. In **statistical (data) analysis** people are interested in analysing the properties of a given data set. Say you have obtained questionnaires from 500 faculty members. Then your goal is to make statements about these 500 questionnaires. The scope of your study does not extend beyond those 500 data points and all statements that you make are in principle limited to this data set. Obviously, this is not what people do in research papers. Researchers often try to generalize the results they obtain on their data set to a bigger population, like all university employees or even all of humankind. In the following sections we are going to give some indication for why such generalisations may be justified and at the same time warn you that they are often not.

Finally, there is the field of **prediction**. In prediction you again analyse your data, but what you actually want to do is to predict future data of the same kind. Your current data set is of no actual interest to you except that it allows you to gather information that may turn out to be valuable for making your predictions. Again, if you have compiled 500 questionnaires from faculty, you would like to predict what the rate of alcoholics for the following 100 questionnaires is. After you have extracted the information you need from your original data set, you could even discard it in this setting. In practice, of course, you should NEVER discard your data. Instead, you should make it publicly available, so that other people can reproduce your study.

This latter field of prediction is nowadays most commonly known as **machine learning**. However, statistical analysis and prediction are closely intertwined and share a lot of their methodology. It is therefore not always easy to make the distinction.

## 5.2 Statistics and Sample Means

In the previous section we have introduced the word **statistic** and also alluded to the fact that we often assume that our observed data is distributed according to some distribution. The way we usually conceptualize data is that each data point is an instantiation of a random variable. This means that when you are observing 1000 data points, we conceptualize this as observing the outcomes of 1000 random variables. Importantly, each data point could potentially have taken on a different value and it just so happens that in our specific **data sample** it took on the value that it did.

There is one further assumption that we usually make about our data, namely that it is **i.i.d.** (identical and independently distributed). This just means that we assume that all the random variables that generated our data points follow the same distribution and that they are independent of each other. When we say they follow the same distribution, we do not just mean the same class of distributions (e.g. multinomial), but really the same distribution with identical parameters. We often call that distribution the **data-generating distribution**, but you also find the terms *underlying distribution* or *true distribution* in the literature. We have in fact already used the i.i.d. assumption before. When we do repeated Bernoulli trials (as in Section 3.4), the total probability of the resulting sequence is computed as a product of independent RVs. We can encode the i.i.d. assumption for $n$ Bernoulli trials as follows:

$$\forall i \text{ s.t. } 1 \leq i \leq n : X_i \sim \mathit{Bernoulli}(\theta)\,. \tag{5.1}$$

All $X_i$ follow the same distribution since the parameter $\theta$ does not depend on $i$ but is constant throughout. By the same token, we get independence as the distribution does also not depend on other RVs. Thus, repeated Bernoulli trials, such as repeated coin flips, do actually invoke the i.i.d. assumption. When working with real data this assumption will often be violated but we are going to make it nonetheless for mathematical convenience or if we can motivate it based on our knowledge of the data set.

After we have described our conception of data, let us move on to defining what a statistic is.

**Definition 5.1** *A* statistic *is the value of any function of a data sample. If we have sampled* $n$ *data points that we assume are instantiations of RVs* $X_1^n$*, a statistic is the value of a function* $g$ *on those RVs, i.e.* $g(X_1^n)$*.*

Arguably the most important statistic in all of statistics is the **sample mean**. The sample mean is just the average of the values of the RVs $X_1^n$, i.e. of the data points. It is usually denoted by $\overline{\mu}$. The sample mean can be seen as guess of the expectation of $X_i$. The expectation is sometimes also called mean and $\overline{\mu}$ estimates it from a data sample; hence the name sample mean. Some distributions even have their mean $\mu$ as a parameter. To indicate that we are just making a guess at $\mu$ we put a horizontal bar on top. This same indicator (or a similar one, like a caret, in which case we would write $\hat{\mu}$) can be used for other quantities, as well.

**Definition 5.2** *The sample mean of i.i.d. random variables* $X_1, \ldots, X_n$ *is defined as*

$$\overline{\mu} := \frac{1}{n}\sum_{i=1}^{n} X_i \ .$$

Notice that since $\overline{\mu}$ is the average of a collection of random variables, it is itself a random variable. Thus, we can compute its expectation.

$$\mathbb{E}[\overline{\mu}] = \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n} X_i\right] \tag{5.2}$$

$$= \frac{1}{n}\mathbb{E}\left[\sum_{i=1}^{n} X_i\right] \tag{5.3}$$

$$= \frac{1}{n} \times n\mathbb{E}[X] \tag{5.4}$$

$$= \mathbb{E}[X] = \mu \tag{5.5}$$

This result is huge! Before we interpret it, let us be clear about how we computed it: lines (5.3) and (5.4) follow from the linearity of expectation and the fact that the RVs are i.i.d.

So why is this result so important? It says that the expectation of the sample mean is equal to the true mean. This means that sampling data gives us a way to estimate the true mean. Since the sample means are random variables and therefore distributed according to some distribution, each sample mean should show up in proportion to its probability. Thus, the mean of sample means will approximate the true mean. Conceptually this may be quite a bit to chew on, but the practical implications are compelling. If you are running one experiment (i.e. if you take one data sample) you basically have no clue how probable that sample mean is according to the distribution of sample means. It could be very improbable and thus not be representative at all of the population you are investigating. So what should you do? The above result tells us that you should just repeat your experiment *enough* times, so that you get *enough* sample means. The mean of those sample means will in turn be pretty close to the true mean of the distribution that underlies your population of interest. This is the mathematical reason why in science we want our experimental results to be replicable. If I get a result and several other people get the same or reasonably close results, we can be fairly sure that we obtained them from a high-probability region in the distribution of sample means, i.e. the results are indeed representative for the population under scrutiny.

**Exercise 5.3** *Under this link you find a file that contains 1000 random samples from a binomial distribution with parameter $n = 100$. The file contains 1000 numbers and the $i^{th}$ number is number of successes in the $i^{th}$ sample. Write a Python script that computes an approximation to the parameter $\theta$ of the binomial.*

We have just said that repetition of results is the gold standard in science because if several sample means are close to each other, each one of them (and their average) is likely to be a reasonable approximation to the true mean of the underlying distribution. Unfortunately, more often than not, we only draw one data sample and thus only have one sample mean. The natural question to ask is whether we can somehow ensure that this one sample mean is informative about the true mean. The strict answer is no. We can always be unlucky and obtain a very improbable and thus non-representative sample mean. On the bright side, we can take measures to reduce or chance of being unlucky (and thereby make the one sample mean more trustworthy). What these measures are is explained in Section 5.4. Let us first review the concept of limits in preparation for the proofs that we are going to see in that Section.

## 5.3 Limits

To help our understanding of the theorem in Section 5.4 we have to recall how mathematical limits are defined. For an infinite sequence of numbers we can ask ourselves whether the sequence will eventually come close to a single point or whether it will just keep moving through the space of real numbers. This question can be formalized with the concept of limits.

**Definition 5.4 (Finite Limit of a sequence)** *Take any sequence of real numbers $(a_n)$ where $a_n := a(n)$ for some function $a : \mathbb{N} \to \mathbb{R}$. We say that $L \in \mathbb{R}$ is the* limit *of that sequence as $n$ goes to infinity if for any $\varepsilon > 0$ we can find an $n_0 \in \mathbb{N}$ such that for any $n \geq n_0$*

$$|L - a_n| \leq \varepsilon \ .$$

*We write $\lim_{n\to\infty} a_n = L$ to express this fact.*

**Definition 5.5 (Infinite Limit of a sequence)** *Take any sequence of real numbers $(a_n)$. We say that the sequence diverges (to $\pm\infty$) if for every $K \in \mathbb{R}$ there is an $n_0 \in \mathbb{N}$ such that for all $n > n_0$ it holds that*

$$|a_n| \geq K \ .$$

*We write $\lim\limits_{n\to\infty} a_n = \pm\infty$ to express this fact.*

Definition 5.4 tells us that if a sequence converges to a limit $L$, then for all but finitely many elements (those at the beginning of the sequence) the difference between each element and $L$ will be $\leq \varepsilon$. More informally, we can say that the difference between the elements of the sequence and $L$ can be made arbitrarily small if we are willing to walk far enough down the sequence. Definition 5.5 has been included for completeness' sake but will not be of much relevance in the remainder of the course.

Notice that it is possible that a sequence has no limit at all (neither finite nor infinite). We will not deal with this case here, though.

**Example of a limit calculation** To give you some more feeling for limits, here is an example. Consider the sequence $a_n = \frac{1}{n}$. What is its limit? Intuitively, $a_n$ becomes smaller as $n$ becomes larger. Moreover, all $a_n$ are non-negative. A good guess for the limit thus seems to be $L = 0$. Let us show that it is indeed the limit of this sequence. Choose any real $\varepsilon > 0$. Then for $n \geq n_0$ we want that

$$|L - a_n| = |a_n| = \frac{1}{n} \leq \varepsilon \tag{5.6}$$

We solve this inequality to get $n \geq {}^1\!/\!_\varepsilon$. Thus we set $n_0 = \lceil {}^1\!/\!_\varepsilon \rceil$ which is the smallest integer $n_0 \in \mathbb{N}$ such that ${}^1\!/\!_\varepsilon \leq n_0$. Since $\varepsilon$ was chosen arbitrarily we conclude that indeed $\lim\limits_{n\to\infty} \frac{1}{n} = 0$. □

Instead of limits of sequences, we will actually need limits of functions. However, notice that limits of functions are simply the limits of sequences of function outputs.

**Definition 5.6 (Limit of a function)** *Consider a function $f$ that is defined on the reals. We say that the limit of $f(x)$ as $x$ approaches $x_0$ is $L$ if for every $\varepsilon > 0$ there exists a $\delta > 0$ such that $0 < |x - x_0| \leq \delta$ implies*

$$|L - f(x)| \leq \varepsilon \ .$$

*We write $\lim\limits_{x\to x_0} f(x) = L$ to express this fact.*

## 5.4 The Weak Law of Large Numbers

The weak law of large number states that as we increase our sample size, the probability tends to 0 that our estimated mean $\overline{\mu}$ will be further than a small amount $\varepsilon$ away from the true expectation $\mathbb{E}[X]$ of the data-generating distribution $P_X$. In other words, the more sample points we take, the smaller is the chance that we commit a large error when estimating the mean from our sample. To become clear about what we need to prove, let us first state the weak law of large numbers.

**Theorem 5.7 (Weak law of large numbers)** *For $n \in \mathbb{N}$, let $X_1^n$, be i.i.d. distributed random variables with distribution $P_X$, expectation $\mathbb{E}[X] \in \mathbb{R}$ and variance $var(X) = \sigma^2 \in \mathbb{R}$. Further let $X_1^n$ have sample mean $\overline{\mu} = \frac{1}{n}\sum\limits_{i=1}^{n} X_i$. Then for any real $\varepsilon > 0$, it holds that*

$$\lim_{n\to\infty} P(|\mathbb{E}[X] - \overline{\mu}| \geq \varepsilon) = 0 \ .$$

At this point it may be good to just pause for a moment, stare at the theorem and try to connect it to the verbal explanation from above. The significance of the theorem derives from the fact that it basically provides us with the theoretical underpinning that allows us to draw inferences from data.

In order to prove the weak law of large numbers, we use two auxiliary lemmas. Once we have proven those, Theorem 5.7 will follow easily.

**Lemma 5.8 (Markov's inequality)** *For any random variable $X$ and any $a > 0$ it holds that*

$$P(|X| \geq a) \leq \frac{\mathbb{E}[|X|]}{a} \ .$$

**Exercise 5.9** *Prove Markov's inequality.*

Besides having established Lemma 5.8, Andrey Markov has made many significant contributions to probability theory. For example, if you go on to study information theory and/or any computational linguistics courses, you are guaranteed to encounter Markov chains. For now, let us move on to our second auxiliary lemma.

**Lemma 5.10 (Chebyshev's inequality)** *Let $X$ be a RV with expectation $\mathbb{E}[X]$ and variance $var(X) = \sigma^2 \in \mathbb{R}$. Furthermore, let $\varepsilon > 0$.*

*Then*

$$P(|\mathbb{E}[X] - X| \geq \varepsilon) \leq \frac{\sigma^2}{\varepsilon^2} \ .$$

**Proof of Lemma 5.10** By Markov's inequality we have that

$$P((\mathbb{E}[X] - X)^2 \geq \varepsilon^2) \leq \frac{\mathbb{E}[(\mathbb{E}[X] - X)^2]}{\varepsilon^2} = \frac{var[X]}{\varepsilon^2} = \frac{\sigma^2}{\varepsilon^2} \ . \tag{5.7}$$

□

The final step in proving the weak law of large numbers is to apply Chebyshev's Inequality in the case where the random variable of interest is the sample mean.

**Proof of Theorem 5.7** We assume i.i.d. RVs $X_1^n$ with sample mean $\overline{\mu} = \frac{1}{n}\sum_{i=1}^{n} X_i$. This means that $\mathbb{E}[X] - \overline{\mu}$ is a RV depending on $X_1^n$ whose variance is

$$\begin{aligned} var(\mathbb{E}[X] - \overline{\mu}) &= var(\overline{\mu}) && (5.8)\\ &= var\left(\frac{1}{n}\sum_{i=1}^{n} X_i\right) && (5.9)\\ &= \frac{1}{n^2} var\left(\sum_{i=1}^{n} X_i\right) && (5.10)\\ &= \frac{1}{n^2}\ n\ var(X) = \frac{var(X)}{n} \ . && (5.11)\end{aligned}$$

Chebyshev's Lemma 5.10 then implies that

$$\lim_{n \to 0} P(|\mathbb{E}[X] - \overline{\mu}| \geq \varepsilon) \leq \frac{\sigma^2}{n\varepsilon^2} \ . \tag{5.12}$$

If we fix $\varepsilon > 0$ and increase $n$, the number of i.i.d. samples, this probability will go to 0. More formally, choose $\delta > 0$. One way to show $P(|\mathbb{E}[X] - \overline{\mu}| \geq \varepsilon)$ to be smaller than $\delta$, is to show $\frac{\sigma^2}{n\varepsilon^2} < \delta$ which happens whenever $\frac{\sigma^2}{\delta\varepsilon^2} < n$. Thus, if we sample more than $\frac{\sigma^2}{\delta\varepsilon^2}$ data points, we can ensure that $P(|\mathbb{E}[X] - \overline{\mu}| \geq \varepsilon) < \delta$. Since $\delta$ is arbitrary, this shows that $\lim_{n \to \infty} P(|\mathbb{E}[X] - \overline{\mu}| \geq \varepsilon) = 0$, which is exactly what the weak law of large numbers states. □

The proof of the weak law of large numbers also sheds some new light on the importance of the variance of the underlying distribution. We want that variance to be as small as possible since we then need fewer samples in order to have a close estimate of the true mean of the data-generating distribution.

Thus, it is helpful if the variance of the data-generating distribution is small. Otherwise we need a lot of samples.

Notice also the relationship between the variance $\sigma^2$ and the number of samples $n$ in the above proof. For a fixed variance, the probability $P(|\mathbb{E}[X]-\overline{\mu}| \geq \varepsilon)$ reduces by a factor that is proportional to $n$. Hence, we need to take more and more samples as we want to decrease the probability that the sample mean deviates from the actual mean by more than $\varepsilon$.

A more common and more practical interpretation of the relationship between $\sigma^2$ and $n$ is the following: suppose we have collected $n$ data points where $n$ is fixed, meaning we have no quick and cheap way to obtain more data points. Then the lower the variance of the data-generating distribution, the more confident we can be that $\overline{\mu}$ is a reasonably good estimate of the true mean of the data-generating distribution. This insight also establishes a relationship to the expectation of sample means (see Equations (5.2)-(5.5)). If the distribution of sample means has low variance, the interval of sample means that are likely to occur is relatively tight. Thus we will only need few sample means in order to compute a good approximation to the true mean.

To visualise the effect of the sample size for a fixed variance, let us take a look at Figure 5.1. The plot on the top shows the same function applied to different data samples from the same distribution, all of which are of relatively small size. The plots therefore show large spread as witnessed by the width of the curves. The plot at the bottom shows the same function applied to a larger data set. One clearly sees that the spread is much smaller.

## 5.5 Sufficient Statistics

A popular interpretation of statistics is that they are data summaries. Obviously, some statistics summarize the data better than others. For example, the constant function $\mathbf{6}(\cdot)$ which returns the value 6 on all inputs delivers an extremely poor summary of most data (in fact it is not sensitive to the data at all). The mean is a more useful summary as it captures some overall tendency in the data.

Is there any statistic that captures all the necessary information in the data? This questions is hard to answer in general but when it comes to capturing the information about the parameters of the underlying distribution, the answer is yes[1]. If a statistics conveys all the information about the parameters that the data contain, we call it a **sufficient statistic**. The formal definition is somewhat less obvious.

**Definition 5.11 (Sufficient Statistics (discrete))** *Given some discrete RV $X$ over data and a statistical model with parameters $\theta$, a statis-*

[1] At least for the distributions that we are concerned with in this script, which are all in the exponential family.

*tic $t(x)$ is sufficient if $P(X = x|t(X) = t(x), \Theta = \theta)$ does not depend on $\theta$, i.e. if*

$$P(X = x|t(X) = t(x), \Theta = \theta) = P(X = x|t(X) = t(x)) \; .$$

The above definition captures exactly what it means for a statistic to contain all the information about the parameters. Once we know the sufficient statistic, we can simply ignore the parameters. As an example, consider the Bernoulli distribution. For set of i.i.d Bernoulli trials $x = x_1^n$, the statistic $t(x) = \sum_{i=1}^n x_i$ is sufficient. To see this, consider the distribution $P(X| \sum_{i=1}^n x_i, \Theta = \theta)$. It takes the following form

$$P\left(X = y| \sum_{i=1}^n x_i, \Theta = \theta\right) = \begin{cases} 0 & \text{if } \sum_{i=1}^n y_i \neq \sum_{i=1}^n x_i \\ \frac{1}{\binom{k}{n}} & \text{otherwise, where } k = \sum_{i=1}^n x_i \end{cases}$$

Clearly, neither of the two left-hand-side terms depends on $\theta$. Thus, $t(x) = \sum_{i=1}^n x_i$ is a sufficient statistic according to our definition. Notice that the sum does not capture the order in which the events occurred. This shows that the sufficient statistic is not a perfect summary in general (after all, we might care about the order of events). It only captures all the information about the parameters that the data contain.

A statistic that is non-sufficient for the Bernoulli distribution is the value of the first outcome, i.e. $t(x) = x_1$. There are several binary sequences that have the same starting value but different numbers of ones and zeros. The corresponding conditional distribution is

$$P(X = y|x_1, \Theta = \theta) \begin{cases} = 0 & \text{if } y_1 \neq x_1 \\ \propto \binom{k}{n}\theta^k(1-\theta)^{n-k} & \text{otherwise, where } k = \sum_{i=1}^n x_i \end{cases}$$

where the proportionality follows because we need to renormalise the probability to all those sequences whose starting values is equal to $x_1$. The crucial point, however, is that the parameter shows up in the right hand side and thus $x_1$ is not a sufficient statistic for the binomial distribution.

**Exercise 5.12** *Assume a RV $X = X_1^n$ whose observations are i.i.d. according to a Poisson distribution with parameter $\lambda$. Recall that the p.m.f. of the Poisson distribution for one data point is*

$$P(X = x|\Lambda = \lambda) = e^{-\lambda}\frac{\lambda^x}{x!} \; .$$

*Show that $t(x) = \sum_{i=1}^n x_i$ is a sufficient statistic for the Poisson distribution as well.*

Definition 5.11 is constrained to discrete distributions. It is also not very useful when one does not yet know the sufficient statistics and has to find them. We will remedy both these problems with the following theorem.

**Theorem 5.13 (Factorisation Theorem)** *Assume a discrete RV over data $X$ and a statistical model $P(X = x|\Theta = \theta)$ with parameters $\theta$. A statistic $t(X)$ is sufficient if and only if the model can be written as*

$$P(X = x|\Theta = \theta) = g(\theta, t(x)) \cdot h(x, t(x)) \ .$$

**Proof** Assume $t(x)$ is sufficient. Then

$$\begin{aligned}
&P(X = x|\Theta = \theta) = P(X = x, t(X) = t(x)|\Theta = \theta) && (5.13)\\
&\quad = P(X = x|t(X) = t(x), \Theta = \theta) \cdot P(t(X) = t(x)|\Theta = \theta) && (5.14)\\
&\quad = P(X = x|t(X) = t(x)) \cdot P(t(X) = t(x)|\Theta = \theta) && (5.15)\\
&\quad = h(x, t(x)) \cdot g(\theta, t(x)) \ ,
\end{aligned}$$

where in (5.13), we used the fact that $t(\cdot)$ is a deterministic function, the second equality is the chain rule and in (5.15), we use that $t(x)$ is sufficient. Now assume that $P(X = x|\Theta = \theta) = g(\theta, v(x)) \cdot h(x, v(x))$ for some statistic $v(x)$. We need to show that $v(x)$ is sufficient in the sense of Definition 5.11. Observe that $P(X = x, V(X) = v(x)|\Theta = \theta) = P(X = x|\Theta = \theta)$ since $v(\cdot)$ is deterministic. Thus

$$\begin{aligned}
&P(v(X) = v|\Theta = \theta) = \sum_{x:v(x)=v} P(X = x, v(X) = v|\Theta = \theta) && (5.16)\\
&= \sum_{x:v(x)=v} P(X = x|\Theta = \theta) = \sum_{x:v(x)=v} g(v, \theta)h(x, v)
\end{aligned}$$

where the last equality follows from our assumption that the p.m.f. of $X$ can be rewritten in the desired way. We now use the p.m.f. for $v(x)$ in the next step.

$$\begin{aligned}
&P(X = x|v(X) = v, \Theta = \theta) = \frac{P(X = x, v(X) = v|\Theta = \theta)}{P(v(X) = v|\Theta = \theta)} && (5.17)\\
&= \frac{P(X = x|\Theta = \theta)}{P(v(X) = v|\Theta = \theta)} && (5.18)\\
&= \frac{g(\theta, v)h(x, v)}{\sum_{x:v(x)=v} g(v, \theta)h(x, v)} = \frac{h(x, v)}{\sum_{x:v(x)=v} h(x, v)} && (5.19)
\end{aligned}$$

Clearly, the conditional does not depend on $\theta$ and thus $v(X)$ is sufficient. □

Now that we have shown the factorisation theorem for discrete RVs we will use it as a general definition for sufficiency, thereby also including continuous RVs.

**Definition 5.14 (Sufficient Statistic)** *Given some RV $X$ over data and a statistical model with parameters $\theta$, a statistic $t(x)$ is sufficient if $P(X = x|t(X) = t(x), \Theta = \theta)$ can be written as*

$$P(X = x|\Theta = \theta) = g(\theta, t(x)) \cdot h(x, t(x)) \ .$$

## 5.6 Parameter Estimation

It is time for us to meet Sir Ronald Fisher, one of the founding fathers of statistics. Many of the methods that Fisher introduced for statistical testing and **parameter estimation** are still in wide-spread use today. One of his biggest achievements was proposing the **Maximum Likelihood Principle**. To understand this principle, we first have to introduce likelihood functions.

Recall that we can informally write Bayes' Rule as

$$\text{posterior} \propto \text{likelihood} \times \text{prior} \ .$$

Recall further that every distribution $P_X$ that we have seen so far depends on a number of parameters. Once these parameters are set, we can compute the probability of any event that is captured by a value of the RV $X$. But what can we do if the parameters are not known? It turns out that we can estimate them. In order to estimate our parameters, we will make the dependence of $P_X$ on its parameters explicit by letting

$$P(X = x) = P(X = x|\Theta = \theta) \ . \tag{5.20}$$

This means we regard $\Theta$ itself as a random variable (over parameters) and use the distribution $P_{X|\Theta=\theta}$ instead of $P_X$. Notice that for all $x$ we have $P(X = x) = P(X = x|\Theta = \theta)$ as long as the parameters of $P_X$ are set to $\theta$. Again, the purpose of this substitution is to make the dependence of the distribution on its parameters explicit.

**Definition 5.15 (Likelihood Function)** *For $n \in \mathbb{N}$ and a* fixed *set of $n$ data points or observations $x = x_n^1 = x_1, x_2, \ldots, x_n$, we define the* likelihood function *of a family of distributions $P_{x|\Theta}$ as*

$$L_x(\theta) := P(X = x|\Theta = \theta) \ .$$

There are two crucial things to note about the likelihood function. First, the data set $x$ is assumed to be fixed. Thus, the only random variable that can take on different values is the parameter RV $\Theta$. This convention also tells us that the likelihood function is a function of the parameters *and not of the data*! This is the reason that we index it with the specific data set $x$ and not with a random variable $X$.

Moreover, the likelihood function is based on conditional probability distributions. If we were to sum over all $x \in \text{supp}(X)$ the result would be one since we would be summing over the support of a distribution with parameter vector $\theta$. Instead, however, the likelihood forces us to leave $x$ fixed and only allows us to sum over all values of $\Theta$. This sum is by no means guaranteed to yield 1 as a result! The important lesson here is that the likelihood function is generally *not a probability distribution*! This is a tough pill to swallow in the beginning and you should maybe take a moment to let this sink in and convince yourself that this is indeed so.

With these (important!) remarks in mind, let us quickly elaborate on notation. Since the data set $x$ is fixed anyway, many authors do not even bother to include it as a subscript of the likelihood function and just write $L(\theta)$. Other authors have adopted the unfortunate convention to write $L(\theta; x)$. While this notation is ok when you know what they are talking about, it may also give you the wrong impression that $x$ is an argument of the likelihood function.

Furthermore, we have made the choice to represent the dependence of the distribution on its parameters as $P(X = x|\Theta = \theta)$. This is the Bayesian way of writing the dependence. A frequentist statistician would rather write $P(X = x; \theta)$ which reads as "the probability of $x$ parametrised by $\theta$". The crucial difference is that the frequentist would feel uncomfortable to regard the parameters $\theta$ as a realisation of a random variable because he would claim not to know how to find "the correct distribution" $P_\Theta$ for that RV.

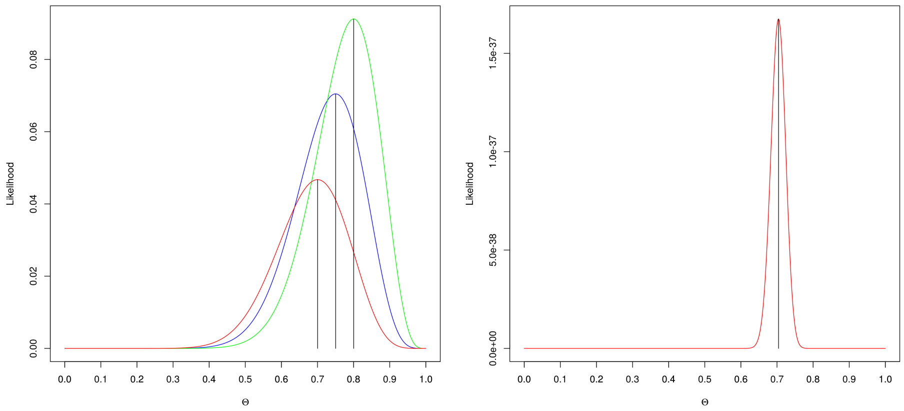
The Bayesian statistician, on the other hand, wants to do exactly that: he wants to impose a distribution $P_\Theta$ over the parameters. If we look back at Bayes' rule, we see that this distribution $P_\Theta$ would play the part of the prior. If, as in the present case, the prior is a distribution over parameters, we also call it a *parameter prior* or *prior over parameters*. We are siding with the Bayesian view here as it is much easier to interpret and do mathematics with.

After choosing a parameter prior we can compute the posterior distribution over parameters.

$$P(\Theta = \theta|X = x) \propto P(X = x|\Theta = \theta) \times P(\Theta = \theta) \tag{5.21}$$

Notice that we do not compute the distribution $P(\Theta = \theta|X = x)$ itself but rather a quantity that is proportional to it. It turns out that this proportional quantity will be all we need in the remainder of this chapter. Let us emphasize however what makes Bayes' rule so important: it gives us a principled way to compute a distribution over parameters from data!

With the posterior over parameters at hand, we can formulate the parameter inference problem: it is the problem of picking a *good* parameter. Notice that exactly this learning problem is referred to when people talk about machine learning. What the machine is trying learn from data are



(a)

(b)

Figure 5.1: Plots of likelihood functions for different data samples. All data samples were randomly drawn from a binomial distribution with parameters $n = 10$ and $\theta = 0.7$. Figure 5.1a depicts the likelihood functions for data samples consisting of 2 draws each. The vertical lines indicate at which value of $\theta$ the likelihoods reach their maximums. Two draws contain relatively little information about the underlying distribution and thus the likelihood function is fairly spread, indicating that there are several parameter values that are about equally good. Figure 5.1b shows the likelihood function for a data sample consisting of 50 draws. 50 draws convey much more information about the underlying distribution and therefore the likelihood function is peaked around the MLE (which is also close to the true parameter 0.7. Deviating slightly from the MLE in his scenario leads to a huge drop in likelihood, effectively ruling out a huge part of the parameter space as candidates for the true parameter.

*good* parameters. Where the statistician would talk about **parameter estimation**, the computer scientist talks about parameter learning. Both expressions refer to the same thing, but machine learning just sounds a lot sexier, doesn't it?

We are left with the question what *good* parameters are. This question does not have a single definitive answer and is actually a constant matter of debate. We are going to present one classic (and still very relevant) answer which is given by the maximum likelihood principle.

## 5.7 The Maximum Likelihood Principle

The maximum likelihood principle simply states that we should try to maximize the likelihood function of our data, that is, we should pick the parameter value that achieves this maximisation. This parameter value is known as the **maximum likelihood estimate** (or as maximum likelihood estimates if there are several).

**Definition 5.16 (Maximum Likelihood Estimate)** *A maximum likelihood estimate (MLE) for a parameter set* $\mathrm{supp}(\Theta)$ *on a data sample* $x$ *is a value* $\theta^*$ *such that*

$$\theta^* = \arg\max_{\theta} L_x(\theta)$$

In Figure 5.1 we have plotted some likelihood functions. They are based on data samples that were randomly generated from a binomial distribution with parameters $n = 10$ and $\theta = 0.7$. The likelihood plots in Figure 5.1a are based on data sets of only two samples, that is 20 i.i.d. Bernoulli trials. The plot in Figure 5.1b is based on a data set of 50 samples, that is 500 i.i.d. Bernoulli trials. The vertical lines connect the maximum likelihood estimate for each data set with its likelihood value. Notice the different scales of the two plots. The likelihood value depends on the data size. Therefore, it does not make sense to compare likelihood values across data sets. After all, each data set comes with its own likelihood function and the likelihood functions of different data sets are indeed different functions. This difference is also the reason why the maximum likelihood principle tells us to only find the parameter value $\theta$ at which the maximum of the likelihood function is achieved. There is no point in even looking at the numerical likelihood value of that maximum.

Notice further that in Figure 5.1, there is only one MLE for each of these functions. We will shortly see why it is desirable for the likelihood function to only have one maximum.

Let us explain how to compute a MLE. By definition, the likelihood function maps the MLE to one of its maximums. From calculus we know that the derivative of any differentiable function is 0 at the function's maximums[2]. Hence, all we need to do in order to find the MLE is to differentiate the likelihood function with respect to $\theta$ and check where the derivative is 0. First, however, we need to write down the likelihood function. Looking back at Definition 5.15, we recall that the likelihood is defined only with respect to a probabilistic model. In order to write down a likelihood function, we need to first define such a model. In other words, we have to define concrete likelihood functions on a case-by-case basis. We present one such case as an example below. Before we do so, let us note that for mathematical convenience, one often uses the logarithm of the likelihood function instead of the likelihood function itself. Taking the logarithm has two advantages:

[2] Technically we also require that the function be defined on a closed (as opposed to open) interval. At this stage it is ok to assume that our parameter sets are always closed intervals.

1) logarithms turn products into sums and sums are often easier to handle and 2) when using a computer, very small values may be rounded down to 0. Logarithms mitigate this problem as they turn very small numbers into negative numbers that have rather large absolute values.

**Definition 5.17 (Log-Likelihood)** *For $n \in \mathbb{N}$ and a* fixed *set of $n$ data points or observations $x = x_n^1 = x_1, x_2, \ldots, x_n$, we define the log-likelihood function over a family of distributions $P_{x|\Theta}$ as*

$$\mathcal{L}_x(\theta) := \log\left(L_x(\theta)\right) \ .$$

Notice that finding the maximum of the logarithm of any function $f$ that only takes on positive values is the same as finding the maximum of the original function $f$. This is so because the logarithm function is strictly increasing, meaning that for any two possible arguments $x > y > 0$, we have $\log(x) > \log(y)$ and hence, if $f(w) > f(z)$, we have $\log(f(w)) > \log(f(z))$.

In order to make it easier to find MLEs of your own, we give you a procedure that you can apply in most cases and show you an example of how to use it.

1. Define a probabilistic model.
2. Write down the functional form of $L_x(\theta)$ for the parameters of that model.
3. Write down $\mathcal{L}_x(\theta)$.
4. Compute $\frac{d}{d\theta}\mathcal{L}_x(\theta)$. This is also called the score function.
5. Solve $0 = \frac{d}{d\theta}\mathcal{L}_x(\theta)$ for $\theta$.

**Example of finding the MLE** Assume we have to do market research for a clothing store in Amsterdam. The store wants to expand its size and the manager wonders whether he should use the extra space to exhibit more men's or more women's clothing. To help him with this decision, we are going to count how many male and female customers are coming in on a given day. We treat the gender of each of the $n$ customers as a random variable $X_i$ and interpret $X_i = 0$ as male and $X_i = 1$ as female. We assume that the underlying distribution that determines the gender of customers is the same for all customers. We also assume that a customer's gender is independent of the gender of any other customer. Hence, we stipulate that $X_i \perp X_j$ whenever $i \neq j$.

As an aside, notice that these assumptions are not without problems in real applications. The first assumption, that the gender distribution is the same for all customers, may not always be justifiable. Depending on the time of the day, it is possible that more men or women will come in. The second assumption, that the gender of one customer does not depend on the gender of other customers, may also not always be true. If couples come to shop at the store, then the gender of one partner will determine the gender of the other partner (in which way the partners in a couple determine each other's genders depends on whether the couple is homo- or heterosexual). For the sake of the example we will nevertheless assume that our assumptions hold true.

**Step 1:** As the day is over, we have observed $k$ women and $n-k$ men. Above, we postulated a model according to which the occurrences are distributed according a binomial distribution whose parameter $n$ we already know: it is simply the total number of our observations (a.k.a. the total number of customers who entered the shop that day). What we want in order to facilitate the manager's decision is to estimate $\theta$, the probability that a random customer is female.

**Step 2:** Our likelihood function looks as follows:

$$L_x(\theta) = \binom{n}{k}\theta^k \times (1-\theta)^{n-k} \; . \tag{5.22}$$

As a mnemonic that $\theta$ is unknown we can informally write

$$L_x(\theta) = \binom{n}{k}?^k \times (1-?)^{n-k} \; .$$

**Step 3:** We can now take the logarithm of our likelihood function.

$$\begin{align} \log(L_x(\theta)) &= \log\left(\binom{n}{k}\theta^k \times \theta^{n-k}\right) \tag{5.23} \\ &= \log\left(\binom{n}{k}\right) + k\log(\theta) + (n-k)\log(1-\theta) \tag{5.24} \end{align}$$

**Step 4:** To find the MLE, we first differentiate the log-likelihood with respect to $\theta$.

$$\begin{align} \frac{d}{d\theta}\mathcal{L}_x(\theta) &= \frac{d}{d\theta}\log\left(\binom{n}{k}\right) + k\frac{d}{d\theta}\log(\theta) + (n-k)\frac{d}{d\theta}\log(1-\theta) \tag{5.25} \\ &= \frac{k}{\theta} - \frac{n-k}{1-\theta} \tag{5.26} \end{align}$$

**Step 5:** Finally, we want to find a point where this derivative vanishes in order to find the maximum of $\mathcal{L}_x$.

$$0 = \frac{k}{\theta} - \frac{n-k}{1-\theta} \quad \Leftrightarrow \tag{5.27}$$

$$\frac{n-k}{1-\theta} = \frac{k}{\theta} \quad \Leftrightarrow \tag{5.28}$$

$$(n-k)\theta = k(1-\theta) \quad \Leftrightarrow \tag{5.29}$$

$$n\theta - k\theta = k - k\theta \quad \Leftrightarrow \tag{5.30}$$

$$n\theta = k \quad \Leftrightarrow \tag{5.31}$$

$$\theta = \frac{k}{n} \tag{5.32}$$

And we are done! You know once and for all that the MLE for the parameter $\theta$ of *any* binomial distribution with parameter $n$ (and having observed $k$ occurrences) is $\frac{k}{n}$.

**Exercise 5.18** *A coin is getting flipped 1000 times and comes up heads 600 times. According to the MLE, would you say that this coin is fair?*

Those who are already familiar with calculus may have felt a bit uncomfortable, because we simply state that setting the derivative of the log-likelihood to 0 will give us a maximum of that function. In general, this technique will only give us an extremum which might as well be a minimum. How can we be so sure that we really got a maximum? We will just do a proof by picture here and let you do the math.

Take another look at Figure 5.1. Clearly, we only see one maximum per function and that one is unique in all cases. What you cannot see in the plots is that the likelihood is never 0 for any $\theta \in (0, 1)$. It is just really, really small, that is why it looks as if it was 0 in many places in the plot. What actually happens is that the likelihood is constantly decreasing as $\theta$ approaches 0 and 1. This constant decrease implies that the derivative is not equal to 0 anywhere other than at the maximum.

Finally, notice that the likelihood is only equal to 0 when $\theta = 0$ or $\theta = 1$. Thus, the likelihood function does indeed have two minima. However, these occur at the boundary points of the interval $[0, 1]$ and since we just stated that $L_x(\theta)$ is constantly decreasing as $\theta$ approaches those points, we can safely conclude that the maximum does not lie on the boundary points. Hence, the only point at which the derivative of the likelihood function of the binomial distribution is 0 is at the sole maximum.

We have mentioned above that having only one maximum is a desirable property. If we want to find the MLE, we have but one choice in this case. If there were several maxima, we would have to compute all of them and pick amongst them. If there are two maxima that have equal likelihood values, we have no way of choosing between them and thus no way of determining the single best parameter estimate. Moreover, we will encounter situations in the next chapter where it is very hard (if not impossible) to find the global MLE (i.e. the MLE at the highest maximum).

You may rightfully wonder what distributions have the desirable property of only having one maximum in their likelihood functions. It turns out that those are exactly the distributions in the exponential family. The link includes a list of those distributions and you will be happy to see that most commonly used distributions are members of the exponential family and thus their likelihoods only have one maximum. Another feature of exponential family distributions is that they all have sufficient statistics. Hence, whenever we are doing maximum likelihood estimation for an exponential family distribution, all we need to know about the data are the sufficient statistics. This point will become important in the following chapter.

**Exercise 5.19** *You are given some likelihood function $L_x$ for the binomial distribution along with its MLE $\theta^*$. Show rigorously that $\theta^*$ is indeed a maximum. That is, show that $\mathcal{L}_x''(\theta^*) < 0$, where $\mathcal{L}_x''$ is the second derivative of the log-likelihood function.*

## 5.8 Maximum a Posteriori Estimation

Recall that in Section 5.6 we set ourselves the goal of finding a good parameter estimate from the posterior distribution over parameters. Let us say that the best parameter estimate is the one with the highest posterior probability. Then the question is: do we actually accomplish our goal with the MLE? Does the MLE give us the parameter with the highest posterior probability? Unfortunately, the general answer is no, which becomes evident from Bayes' rule.

$$\arg\max_{\theta} P(\Theta = \theta | X = x) = \arg\max_{\theta} P(X = x | \Theta = \theta) \times P(\Theta = \theta) \tag{5.33}$$

The MLE only maximises over the likelihood term but not over the prior! Hence it will in general be different from the **maximum a posteriori** estimate.

**Definition 5.20 (Maximum a posteriori estimate)** *A maximum a posteriori (MAP) estimate for a parameter set* $\text{supp}(\Theta)$ *on a data sample $x$ is a value $\theta^*$ such that*

$$\theta^* = \arg\max_{\theta} P(\Theta = \theta | X = x) \ .$$

The MAP estimate can be derived with exactly the same steps as the MLE. However, parameters are usually real values which means that distributions over them are continuous distributions. Since we have not dealt with continuous distributions in this course, we will stop just short of actually imposing (non-uniform) prior distributions over parameters and computing MAP estimates.

Notice that up to now, we justified the maximum likelihood principle merely from intuition by postulating that high likelihood should somehow be an indicator for good parameter values. We will now justify the maximum likelihood principle more formally, by showing that the MLE is just a special kind of MAP estimate. Since this realisation implies that under certain condition the MLE will also have the highest posterior probability, we can safely argue for the MLE based on its posterior probability.

Let us assume that our prior distribution $P_\Theta$ over parameters is uniform. Then we can write the MAP estimator[3] as

$$\arg\max_{\theta} \frac{\partial}{\partial\theta} \log(P(\Theta = \theta | X = x)) \tag{5.34}$$

$$= \arg\max_{\theta} \frac{\partial}{\partial\theta} \log(P(X = x | \Theta = \theta) \times P(\Theta = \theta)) \tag{5.35}$$

$$= \arg\max_{\theta} \frac{\partial}{\partial\theta} \log(P(X = x | \Theta = \theta)) + \log(P(\Theta = \theta)) \tag{5.36}$$

$$= \arg\max_{\theta} \frac{\partial}{\partial\theta} \log(P(X = x | \Theta = \theta))\,, \tag{5.37}$$

where we used the uniformity of $\Theta$ to get from (5.36) to (5.37). We can neglect $\log(P(\Theta = \theta)$ when finding the maximum, because if we add a constant to all likelihood values, the MLE will not change.

This derivation tells us that if we choose a uniform parameter prior, the MLE will be the MAP estimate. Hence, what we are actually assuming whenever we choose the MLE as our parameter estimate, is that our prior over parameters is uniform. This is a very strong assumption to make and one may rightfully criticise the maximum likelihood principle because of this assumption (actually one should).

Let us conclude this section by saying that for the rest of this course we will make the assumption that we are using uniform parameter priors with justification. This means that we can safely use the MLE in order to find the parameter value with the highest posterior probability.

## Further reading

If your calculus is a bit rusty or you have never taken a calculus class before, you should consult OSU's excellent (and very fun) online course which allows you to learn at your own pace. The course also comes with a lecture script

[3] If you know some continuous probability theory: the MAP estimate is taken on the posterior density function in this case since the distribution over parameters is continuous.

that contains many insightful examples and exercises. Let us emphasise that doing statistics (including machine learning) without a solid understanding of calculus is close to impossible.

If you are looking for a good introduction to parameter estimation that covers everything we have discussed here and also goes a considerable stretch further, we refer you to Gregor Heinrich's widely cited tutorial. Heinrich's examples come from text modelling but the techniques he describes can be applied anywhere. One of the model he discusses, Latent Dirichlet Allocation, originates from text modelling but has wide-spread applications in biology, as well.

# Chapter 6

# The EM Algorithm

## 6.1 Mixture Models

In the previous chapter we have mentioned that it may happen that a likelihood function has multiple maxima and that sometimes it may be hard or impossible to find the global maximum (i.e. the maximum with the overall highest likelihood value). Such a situation occurs whenever the probabilistic model that we use to model our observations is a **latent-** or **hidden-variable model**. Latent-variable models are models that besides modelling observed data also model a portion of unobserved data. For example, if we look at the income distribution of a population we may want to further differentiate between age groups. If the age of all or some members of the population is not provided in the data, we can still model it as a latent variable. The difficulty is that we will have to make inferences about the age of an individual based on other information that we have about it (e.g. the income).

While it may in general be quite hard to formulate latent-variable models, there are certain standard latent-variable models that have wide-spread applications. One such class are **mixture models**.

**Definition 6.1 (Mixture Model)** *We assume jointly distributed random variables $X = X_1^n$ and $Y = Y_1^n$ where $Y$ is categorical (as defined on Page 37) and $supp(Y) = \{c_1, \ldots, c_k\}$. The $X_i$ are observed data, the $Y_i$ are latent or observed and the $c_j, 1 \leq j \leq k$ are called mixture components. If the distribution $P(X_1^n = x_1^n, Y_1^n = y_1^n \mid \Theta = \theta)$ factors as*

$$P(X_1^n = x_1^n, Y_1^n = Y_1^n \mid \Theta = \theta)$$
$$= P(Y_1^n = y_1^n \mid \Theta = \theta) \prod_{i=1}^{n} P(X_i = x_i \mid Y_i = y_i \mid \Theta = \theta) \ .$$

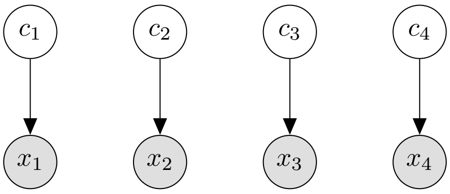


Figure 6.1: A graphical model of the mixture model used in our example. Only four data points are shown. Shaded nodes indicate observed values, light nodes indicate latent values. A graphical model shows the dependencies between variables in a probabilistic model. In this example we see that a) the latent variables are independent of each other and b) the observed variables are independent given the latent variables. (Aside: formally the graphical model actually shows the *independencies* assumed by our model! Reasoning about it in terms of dependencies is often easier, though.)

*we call this model a* mixture model*. The marginal probabilities* $P(Y_i = y_i)$ *for* $1 \leq i \leq n$ *are called* mixture weights*.*

Mixture models are extremely useful whenever we have different ways to think about our data. Each way of conceptualising our data can be encoded by one of the mixture components of the mixture model. The modelling of the data under that view is done by the conditional distribution induced by the mixture component. This technique can help us to build a better overall model of our data. Let us introduce a running example that we use for the rest of this section. A graphical depiction of the model used in the example is given in Figure 6.1.

**Notation** Notice that throughout this chapter we use $\Theta$ as a generic variable over collections of parameters. Assume any model that has parameters $p$ and $q$. Then we have $\Theta = (p, q)$. For the time being you can thus regard the conditioning on $\Theta = \theta$ as an underspecified dependence on any parameters that the model may have. We will become more concrete about parameter values in Section 6.3.

**Example of a mixture model** Assume we observe 20 sequences of coin tosses. Each sequence contains 10 flips. We also know that there are 3 coins with which these sequences could possibly have been generated and for each sequence a different coin may have been used. We want to find out what the biases of the coins are (i.e. the parameters of the binomial distributions associated with the coins) and the probability for each coin to have generated a particular sequence.

We could assume that the entire data set was generated by exactly one coin. We would then employ maximum likelihood estimation to find the parameter of that coin. However, this model might actually turn out to be pretty bad because we are committing to picking one coin only. This is a bad assumption, because we know that each sequence may have been generated by a different coin.

A mixture model comes to the rescue. Instead of assuming that only one coin has generated all 20 sequences, we assume that all three coins have contributed to generating the 20 sequences. However, their contributions may not be equal. This inequality is exactly what the mixture weights capture.

In order to model the contribution of each coin, we introduce a latent RV $Y$ over mixture components with labels $c_1, c_2, c_3$ representing the three coins. In the present case, each mixture component is linked to a binomial distribution, parametrized by the biases of the coins. We will also adopt the often-used assumption that the mixture components are independent of each other. This means that the coin that generated each sequence of coin flips was chosen independently of the coins used for the other sequences. Our independence assumptions are also encoded in the graphical model in Figure (6.1). As usual, we call our data $x$. This information suffices to formulate our mixture model.

$$\begin{aligned} (6.1) \qquad & P(X_1^n = x_1^n, Y_1^n = y_1^n \mid \Theta = \theta) \\ & = \prod_{i=1}^{n} P(Y_i = y_i \mid \Theta = \theta) P(X_i = x_i \mid Y_i = y_i, \Theta = \theta) \end{aligned}$$

Notice that if we were given the mixture weights, estimating the parameters of the mixture components would be easy: we would simply find the MLE for each mixture component separately. The mixture model could then easily be constructed because the mixture weights are known.

Usually, we face a more difficult problem when working with mixture models. Neither the mixture weights nor the parameters of the mixture components are known. In this case, doing straighforward MLE is impossible because the data is incomplete[1].

How can we go about estimating the model parameters, i.e. the parameters of the mixture components and the mixture weights? Each factor in (6.1) is in fact a joint distribution (by the chain rule). We exploit this to rewrite the model as a model of the observed data only.

[1] Incomplete data is another name for a collection of random variables of which some have unobservable (latent) outcomes. Data modelled with a mixture model is incomplete because it contains an observed part (the number of heads in our example) and a latent part (the mixture components which in our example are the types of coin). In general, whenever you have complete data, analytic MLE computation is possible. The moment your data is incomplete, it becomes impossible.

(6.2)

$$
\begin{aligned}
P(X_1^n = x_1^n \mid \Theta = \theta) &= \sum_{j_1=1}^{3}\sum_{j_2=1}^{3}\cdots\sum_{j_n=1}^{3} P(X_1^n = x_1^n, Y_1 = c_{j_1}, \ldots, Y_n = c_{j_n} \mid \Theta = \theta) \\
&= \sum_{j_1=1}^{3}\sum_{j_2=1}^{3}\cdots\sum_{j_n=1}^{3}\prod_{i=1}^{n} P(X_i = x_i, Y_i = c_{j_i} \mid \Theta = \theta) \\
&= \prod_{i=1}^{n}\sum_{j=1}^{3} P(X_i = x_i, Y_i = c_j \mid \Theta = \theta)\,,
\end{aligned}
$$

where the second equality uses the fact that we have assumed independence between the mixture components and hence the expression $P(X_1^n = x_1^n, Y_1^n = y_1^n \mid \Theta = \theta)$ factorizes. Now that we have related mixture models to the probability of the observed data, we can hope to estimate their parameters using the maximum-likelihood principle.

There is one remaining problem, however: if the mixture weights $P(Y_i = y_i)$ are unknown, there is no closed-form solution for estimating the likelihood function. This is because the likelihood depends on the parameters of the mixture components whose distribution, given by the mixture weights, is unknown. This means that while we can compute the likelihood for each individual mixture component, we cannot compute the likelihood of the entire mixture model because we do not know how much each component contributes to the overall likelihood term. As a consequence, we can not simply apply calculus as we have been doing up to now. For this reason, we turn to the **EM algorithm**, that allows to at least find a local maximum of the likelihood function.

One final note: At the beginning we introduced latent-variable models (and hence mixture models) as models of *latent data*. We have cast the problem of inferring the mixture weights as inferring a distribution over mixture components, however. One may argue that those are not data, neither latent nor observed. This is a fair criticism but there is an easy way out. Simply imagine that each sequence of coin flips was annotated with a pointer to the mixture component (the coin) that generated it. This annotation is clearly part of the data. Since in our actual data, these annotations are missing, we treat them as latent data.

## 6.2 The EM Algorithm

In order to estimate the parameters of mixture models, we can employ a classical algorithm of **unsupervised learning**[2], namely the **expectation-**

[2] Whenever the feature of our data that we want to predict (such as the coin which generated a sequence) is observed, we speak of supervised learning. If the target feature

**maximisation (EM) algorithm**. This algorithm allows to find a local maximum of the likelihood function of mixture models or, more generally, models with missing data.

**Another example of latent data.** To give you some more intuition for what latent data is we provide a further example that has spawned a lot of research. Assume you run a website that recommends movies based on a user's preferences. In order to make statistical predictions about what type of user likes what kind of movie, you ask your users to rate movies according to different categories. Say you ask your users to rate the movies for entertainment value, action and fun. What may happen is that some of your users only rate a movie in one or two of these three categories. However, these ratings are still valuable to you and you do not want to throw them away, just because the rating is incomplete. Thus you have a data set with some missing data that you have to fill in somehow.

In mixture models, annotations that tell you which mixture component generated a given data point can be thought of as missing data. As we have seen, such annotations are usually missing and thus we cannot do maximum likelihood estimation. The idea of EM is to make an educated guess at the probability with which each mixture component could *potentially* have generated a data point $x_i$. What we do know is our observed data and some initial guess of the mixture weights which act as prior probabilities for the mixture components (this guess may be arbitrary). Our educated guess is then simply based on Bayes' rule. It is the posterior probability of each mixture component given the data point $x_i$.

Using the posterior over the latent (missing) data, the EM algorithm allows us to probabilistically fill in the missing data and find good mixture weights (where you should understand *good* in the maximum-likelihood sense). The idea behind the algorithm is simple: first, compute the expected number of occurrences of the missing data values (the mixture components). Then treat these expectations as observed and do maximum likelihood estimation as usual[3]. Repeat the procedure until the likelihood does not increase any further. Notice that this procedure requires to fix the number of mixture components in advance.

More formally, assume a data set $X = x$. Furthermore, define $Y$ as a random variable over latent data that can take on $|\mathcal{Y}|$ possible values

is latent, we speak of unsupervised learning.

[3] Notice that expectations can take on non-integer values and thus when treating them as observations we are handling a dataset with "fractional" observations. While this may be conceptually awkward it does not change the mathematics of maximum likelihood estimation.

$c_1, c_2, \ldots, c_{|\mathcal{Y}|}$. Then the likelihood function is

$$L_x(\theta) = P(X = x \mid \Theta = \theta) = \sum_{j=1}^{|\mathcal{Y}|} P(X = x, Y = c_j \mid \Theta = \theta) \tag{6.3}$$

where $\Theta$ ranges over the parameters of the joint distributiforon $P_{XY}$. Recall that EM probabilistically fills in missing data. However, since we are doing maximum likelihood estimation, we are not so much interested in the missing data itself but rather in the sufficient statistics of that data (see Section 5.5). Since we cannot directly obtain the sufficient statistics of missing data, we will instead compute the *expected sufficient statistics*[4].

The EM algorithm is an iterative algorithm, meaning we repeat its steps several times. We use superscripts to indicate the number $l$ of the repetition, where $0 \leq l \leq k$. To formalize the EM algorithm, assume we are at iteration $l$ for which we have some parameter estimate $\theta^{(l)}$ (the initial estimate $\theta^{(0)}$ can be set arbitrarily). Based on this parameter estimate we then compute the expected sufficient statistics of our model which we will call $t(y, x)$.

$$t(y, x)^{(l+1)} = \mathbb{E}(t(Y, x) \mid X = x, \Theta = \theta^{(l)}) \tag{6.4}$$

Equation (6.4) is known as the **E(xpectation)-step** of the EM algorithm. This name comes from the fact that in this step we compute the expected sufficient statistics. To make the algorithm complete, we still miss a **M(aximization)-step**. But that step is simple. We pretend that the expected sufficient statistics of the latent data were actually observed. Once we pretend to observe the expected statistics, the maximization step can be performed using the maximum-likelihood estimation:

$$\theta^{(l+1)} = \arg\max_{\theta} P(X = x, t(Y, X) = t(y, x)^{(l+1)} \mid \theta) \tag{6.5}$$

**Definition 6.2 (EM algorithm)** *We assume a data set $x$ and postulate that there is unobserved data $y$. We also assume a probabilistic model $P(X = x, Y = y \mid \Theta = \theta)$ whose parameters are realisations of a RV $\Theta$. Let $t(x, y)$ be the sufficient statistics for that model. Then any iterative algorithm with $m$ iterations that performs the following steps for $0 \leq l \leq m - 1$,*

***E-step:*** $t(y, x)^{(l+1)} = \mathbb{E}(t(Y, x) \mid X = x, \Theta = \theta^{(l)})$

***M-step:*** $\theta^{(l+1)} = \arg\max_{\theta} P(X = x, t(Y, X) = t(y, x)^{(l+1)} \mid \Theta = \theta)$

[4] Because we are referring to sufficient statistics our exposition of EM is specific to distributions in the exponential family. The EM algorithm can also be made more general. However, since virtually all distributions of interest in practice do belong to the exponential family, we will not make this kind of generalisation.

*to update the model parameters is called an EM algorithm.*

## 6.3 Example of an EM Algorithm for a Mixture Model

Assume as in Section 6.1 that our data is $x = x_1^{20}$ where each $x_i$ is the number of heads that we observed in a sequence of a 10 coin tosses. Again we also assume mixture components representing three coins which are linked to binomials with parameters representing the biases of the coins. The latent data in this case is an annotation that for each observed sequence $x_i$ reveals the coin that has been used to generate that sequence. Thus we have latent data $y = y_1^n$ where each $y_i$ can be one of the three mixture components. We make the additional assumption that choosing a coin to generate a particular sequence is done independently of the coins chosen to generate all the other sequences. This has the effect that in our model the latent data points will be independent[5].

In this example, our collection of parameters $\theta$ consists of two group of parameters, namely $w_1, w_2, w_3$ for the mixture weights and $\phi_1, \phi_2, \phi_3$ which are the parameters of the binomials linked to the mixture components (i.e. these parameters represent the biases of the coins). When we condition on $\theta$, we will often not need all of the parameters in the collection. For example,

$$P(Y = c_1|\Theta = \theta) = P(Y = c_1|W_1 = w_1) = w_1$$

because the first mixture weight is the only parameter that is needed to compute the probability of observing the mixture component $c_1$.

Notice that because the mixture components are categorically distributed we have the constraint that $w_1+w_2+w_3 = 1$. Furthermore because $\phi_1, \phi_2, \phi_3$ are binomial parameters, we know that they have to lie in $[0, 1]$.

**E-step** Initially we arbitrarily assume that the coins have biases of $0.4, 0.5$ and $0.65$, meaning that we initialize the binomial parameters of the data-generating distributions as follows:

$$\phi_1^{(0)} = 0.4 \qquad \phi_2^{(0)} = 0.5 \qquad \phi_3^{(0)} = 0.65 \tag{6.6}$$

We also assume that the fair coin is more likely to be used and hence set its initial mixture weight to $w_2^{(0)} = 0.5$ and the mixture weights of the other two coins to $w_1^{(0)} = w_3^{(0)} = 0.25$ (any other choice would also be fine). Let us take a closer look at our data. To shorten notation, we write it as a list where the i$^{th}$ entry is the value of $x_i$.

$$[6, 5, 4, 2, 2, 6, 5, 5, 4, 2, 5, 2, 4, 4, 6, 4, 5, 6, 3, 3]$$

[5] The assumption that the mixture components in a mixture model are independent is actually quite common.

Then for each $x_i$ we check how likely each coin is to have generated that point. In order to compute the posterior for each coin given a data point, we need the likelihood for that data point. For the first observation we get the following likelihood values.

(6.7)

$$P(X_1 = 6 \mid Y_1 = c_1, \Theta = \theta^{(0)}) = P(X_1 = 6 \mid Y_1 = c_1, \Phi_1 = 0.4) = 0.1114767$$
$$P(X_1 = 6 \mid Y_1 = c_2, \Theta = \theta^{(0)}) = P(X_1 = 6 \mid Y_1 = c_2, \Phi_2 = 0.5) = 0.2050781$$
$$P(X_1 = 6 \mid Y_1 = c_3, \Theta = \theta^{(0)}) = P(X_1 = 6 \mid Y_1 = c_3, \Phi_3 = 0.65) = 0.2376685$$

Recall that the mixture weights are nothing else than priors over mixture components. Hence, in order to get the joint distribution over observed and latent data, we multiply the likelihoods by the mixture weights.

(6.8)

$$P(X_1 = 6, Y_1 = c_1 \mid \Theta = \theta^{(0)}) = 0.25 \times P(X_1 = 6 \mid Y_1 = c_1, \Phi_1 = 0.4) = 0.0278692$$
$$P(X_1 = 6, Y_1 = c_2 \mid \Theta = \theta^{(0)}) = 0.5 \times P(X_1 = 6 \mid Y_2 = c_2, \Phi_2 = 0.5) = 0.1025391$$
$$P(X_1 = 6, Y_1 = c_3 \mid \Theta = \theta^{(0)}) = 0.25 \times P(X_1 = 6 \mid Y_3 = c_3, \Phi_3 = 0.65) = 0.0594171$$

We are ultimately interested in the posterior over mixture components. Because we are dealing with a categorical distribution here, the posterior probability is exactly the expected number of times that each coin has generated data point $x_1$. This is to say that $\mathbb{E}[\mathbb{1}(Y = c_j) \mid X_1 = 6, \Theta = \theta^{(0)}] = P(Y_1 = c_j \mid X_1 = 6, \Theta = \theta^{(0)})$[6]. The posterior given $X_1 = 6$ is shown in Equation (6.9). Recall that we can compute the denominator in Bayes rule (a.k.a. the marginal likelihood) using marginalisation. For example

$$P(X_1 = 6 \mid \Theta = \theta^{(0)}) = \sum_{i=1}^{3} P(X_1 = 6, Y_1 = c_i \mid \Theta = \theta^{(0)}) \; .$$

(6.9)

$$P(Y_1 = c_1 \mid X_1 = 6, \Theta = \theta^{(0)}) = \frac{P(X_1 = 6, Y_1 = c_1 \mid \Theta = \theta^{(0)})}{P(X_1 = 6 \mid \Theta = \theta^{(0)})} = 0.1468149$$
$$P(Y_1 = c_2 \mid X_1 = 6, \Theta = \theta^{(0)}) = \frac{P(X_1 = 6, Y_1 = c_2 \mid \Theta = \theta^{(0)})}{P(X_1 = 6 \mid \Theta = \theta^{(0)})} = 0.5401758$$
$$P(Y_1 = c_3 \mid X_1 = 6, \Theta = \theta^{(0)}) = \frac{P(X_1 = 6, Y_1 = c_3 \mid \Theta = \theta^{(0)})}{P(X_1 = 6 \mid \Theta = \theta^{(0)})} = 0.3130094$$

[6] We use the function $\mathbb{1}(\cdot)$ as an indicator function that evaluates to 1 whenever its boolean argument is true and to 0 otherwise.

| outcome | occurrences | c_1 | c_2 | c_3 |
|---|---|---|---|---|
| 2 | 4 | 0.5674795 | 0.4124300 | 0.0200905 |
| 3 | 2 | 0.4568744 | 0.4980674 | 0.0450583 |
| 4 | 5 | 0.3436451 | 0.5619435 | 0.0944114 |
| 5 | 5 | 0.2370680 | 0.5814960 | 0.1814361 |
| 6 | 4 | 0.1468149 | 0.5401758 | 0.3130094 |

Table 6.1: Posteriors per outcome for the mixture components of the coin flip data set from our EM example.

We compute these expectations over mixture components for each data point and add them up. The reason we can simply add the expectation is that the latent variables are independent and consequently their expectations are independent. If this was not the case, simple adding would not be possible. How exactly the expectations can be accumulated depends on how the model's distribution over latent variables factorises. This has to be handled on a case-by-case basis. For our examples the expectations for each outcome can be found in Table 6.1.

Once the expectations have been added, we need to compute the sufficient statistics for our model. First of all notice that we are dealing with a mixture model where the latent variables are always categorical. Thus, in order to update the parameters of $P_Y$ we need to find the sufficient statistics for a categorical distribution. Recall that these sufficient statistics are simply the counts per outcome observed in the data. Thus the expected sufficient statistics for a categorical are the expected counts per outcome. But these are simply the posterior probabilities! Thus we need to multiply the posteriors per of each observed outcome with the number of times this outcome was seen in the data and sum over all observed outcomes. For mixture component $c_1$ (the first coin with parameter $\phi_1^{(0)} = 0.4$) this gives

$$\begin{aligned} \text{(6.10)} \quad \mathbb{E}(\mathbb{1}(Y = c_1) \mid X = x, \Theta = \theta^{(0)}) &= 4 \times 0.5674795 + 2 \times 0.4568744 \\ &+5 \times 0.3436451 + 5 \times 0.237068 + 4 \times 0.1468149 = 6.6744913 \ . \end{aligned}$$

By parallel calculations we get $\mathbb{E}(\mathbb{1}(Y = c_2) \mid X = x, \Theta = \theta^{(0)}) = 10.5237552$ and $\mathbb{E}(\mathbb{1}(Y = c_3) \mid X = x, \Theta = \theta^{(0)}) = 2.8017535$. These are our expected sufficient statistics. Importantly, we get $\mathbb{E}[\mathbb{1}(Y = c_1) \mid X = x, \Theta = \theta^{(0)}] + \mathbb{E}[\mathbb{1}(Y = c_2) \mid X = x, \Theta = \theta^{(0)}] + \mathbb{E}[\mathbb{1}(Y = c_3) \mid X = x, \Theta = \theta^{(0)}] \approx 20$ (there is some slight numerical imprecision caused by our computer). Notice that this is a useful debugging technique when implementing the algorithm: if the expected number of mixture components does not add up to the number of latent variables in your model, then you almost certainly have a bug in your code!

Next we turn to the sufficient statistics for the binomial distributions linked to the mixture components. These are the counts of the observed outcomes. However, since the binomials are conditional distributions (they are conditioned on the identity of the coins), the counts have to be taken with respect to their conditioning contexts. In other words: we cannot count the observed outcomes independently but we have to count pairs of observed and latent variables. Formally this means that for one binomially distributed observation $x_i$ that $\mathbb{E}[\mathbb{1}\left(X_i = x_i, Y_i = c_j\right) \mid \Theta = \theta^{(0)}] = P(Y_i = c_j \mid X_i = x_i, \Theta = \theta^{(0)})$. This is again just the posterior that we find in Table 6.1.

To get the expectations for the mixture components, we summed the columns in Table 6.1, effectively conflating all outcomes of $X$. We did this because we did not care about $X$ at this stage, only about the expectations of $Y$. When computing the posteriors for the outcomes given the mixture components, we have to sum the posteriors differently. Now we actually need to discriminate between observed outcomes. We only sum over observations that had the same outcome. Working with Table 6.1 this means that we multiply each cell, which contains the posterior for one observation, by the number of times each outcome has been observed in the data set. In other words, we are summing the posteriors over the observations that were equal to the given outcome. For the pairs $(X = 2, Y = c_1)$ and $(X = 4, Y = c_3)$ this gives:

$$\mathbb{E}[\mathbb{1}\left(X = 2, Y = c_1\right) \mid \Theta = \theta^{(0)}] = 4 \times 0.5674795 = 2.269918 \tag{6.11}$$

$$\mathbb{E}[\mathbb{1}\left(X = 4, Y = c_3\right) \mid \Theta = \theta^{(0)}] = 5 \times 0.0944114 = 0.4720569 \tag{6.12}$$

The expected number of times each outcome has been drawn from each coin can be found in Table 6.2.

Recall that the sufficient statistic for the binomial is $\sum_{i=1}^{n} x_i$ where $x_i$ is the $i^{th}$ Bernoulli trial of that binomial. When dealing with $m$ i.i.d. binomial draws, this becomes $\sum_{i=1}^{nm} x_i$. Notice that we do not know $m$ because we don't actually know how many draws stem from each coin. Instead, we use the expected number of times that each coin (mixture component) was used. We have already computed these expectations and noted them down in Table 6.2. Thus, for coin $c_1$ the expected sufficient binomial statistic is

$$\begin{aligned} \mathbb{E}\left[\sum_{i=1}^{nm} x_i \mid c_1\right] &= 2 \times 2.269918 + 3 \times 0.9137487 + 4 \times 1.7182254 \\ & 5 \times 1.1853398 + 6 \times 0.5872594 = 23.6042391 \end{aligned} \tag{6.13}$$

The expected sufficient statistics for all coins are given in Table 6.3.

That we have computed all sufficient statistics for our model means that we have completed the E-step!

**M-step** As pointed out before, the M-step is rather trivial once we have all the necessary expectations. Recall that according to our model, the

| outcome | c_1 | c_2 | c_3 |
|---|---|---|---|
| 2 | 2.2699180 | 1.6497199 | 0.0803621 |
| 3 | 0.9137487 | 0.9961348 | 0.0901165 |
| 4 | 1.7182254 | 2.8097177 | 0.4720569 |
| 5 | 1.1853398 | 2.9074798 | 0.9071804 |
| 6 | 0.5872594 | 2.1607030 | 1.2520376 |

Table 6.2: Posterior expectations of the observed outcomes in the context of each mixture component.

| c_1 | c_2 | c_3 |
|---|---|---|
| 23.60424 | 45.02833 | 14.36743 |

Table 6.3: Expected sufficient statistics for each or the three coins.

mixture components are categorically distributed and thus in the M-step we want to find the MLE of that categorical. In general, the MLE for $w_j$ of a categorical is $\frac{\#c_j}{m}$[7]. In our case $m = 20$. Since we have not observed the latent variables, we simply use their expected sufficient statistics (their expected counts) instead. Thus we set $w_j^{(1)} = \frac{\mathbb{E}[\mathbb{1}(Y=c_j)|X=x,\Theta=\theta^{(0)}]}{20}$[8]. The updated mixture weights then are

$$\begin{aligned} P(Y = c_1 \mid \Theta = \theta^{(1)}) &= w_1^{(1)} = 0.3337246 \\ P(Y = c_2 \mid \Theta = \theta^{(1)}) &= w_2^{(1)} = 0.5261878 \\ P(Y = c_3 \mid \Theta = \theta^{(1)}) &= w_3^{(1)} = 0.1400877 \end{aligned} \tag{6.14}$$

We already know the maximum-likelihood estimate for binomial distributions from Section**??**. The only novelty when it comes to EM for mixture models is that the conditioning contexts are not observed anymore. Again, we fall back on the expected context counts.

For example, if we want to find the conditional distribution for $c_1$, we need to compute the binomial MLE *only for the data associated with* $c_1$! We

[7] This fact can easily be seen by letting $\#c_j$ be the number of successes in the realisation of a binomial RV and the sum of all $\#c_k,\ k \neq j$ be the number of failures. Then clearly $\frac{\#c_j}{m}$ is the MLE.

[8] When implementing the algorithm, numerical imprecisions occur due to the limited memory of our computers. To ensure that the distribution obtained from the M-step really sums to 1, you should use the sum $\sum_{j=1}^{3} \mathbb{E}[\mathbb{1}\,(Y = c_j) \mid X = x, \Theta = \theta^{(0)}]$. This sum should be equal to 20 up to at least the third decimal but may not be exactly equal to 20. Having a distribution that does not exactly sum to 1 may not be to bad after 1 M-step. However, this slightly wrong distribution will then lead to slightly wrong estimates in the E-step. If in the next M-step the distribution does again not sum to 1, the error induced by the numerical imprecision magnifies with each iteration. Therefore you should always divide by $\sum_{j=1}^{3} \mathbb{E}[\mathbb{1}\,(Y = c_j) \mid X = x, \Theta = \theta^{(0)}]$ in order to ensure proper normalisation.

| c_1 | c_2 | c_3 |
|---|---|---|
| 0.3536485 | 0.4278732 | 0.5128013 |

Table 6.4: New parameter values for the binomials associated with each mixture component.

already know from Equation (6.10) that the total expected occurrence of $c_1$ in our data is 6.6744913. You can verify that this is exactly the sum of the first column in Table 6.2. We also know that the MLE for repeated binomial trials is $\frac{\sum_{i=1}^{nm} x_i}{nm}$ where $n$ is the number of Bernoulli trials in each binomial draw (10 in our case) and $m$ is the number of of binomial draws. Since we do not observe the number of draws from $c_1$ our best guess is the posterior expectation. Thus we set $m = 6.6744913$. We also do not directly observe the number of successes per draw from $c_1$ and instead compute the number of expected successes. The number of expected successes happens to be the expected sufficient statistic for the binomial. We have already computed those sufficient statistics in Table 6.3. For coin $c_1$ the binomial MLE is thus

$$\phi_1^{(1)} = \frac{\mathbb{E}\left[\sum_{i=1}^{nm} x_i \mid Y = c_1\right]}{n\mathbb{E}\left[Y = c_1\right]} = \frac{23.6042391}{10 \times 6.6744913} = 0.3536485 \tag{6.15}$$

The updated binomial parameters pre mixture component are given in Table 6.4. This completes our parameter updates and thus the M-step. We can start the next round of estimation by doing the E-step using the updated parameters $\theta^{(1)}$. We will stop iterating when the parameters do not change anymore or after a pre-specified number of iterations.

## Further reading

A great tutorial on EM is provided by Michael Collins who uses Naïve Bayes as a running example. If you want to delve deeper into the theory behind EM and see how it can be interpreted from an information-theoretic perspective, have a look at this classic paper. The daring ones amongst you may also want to consult the original EM paper. Be cautious of he notation they use which is very different from the notation used in this script.

# Chapter 7

# Basics of Information Theory

When we talk about *information*, we often use the term in qualitative sense. We say things like *This is valuable information* or *We have a lack of information*. We can also make statements about some information being more helpful than other. For a long time, however, people have been unable to quantify information. The person who succeeded in this endeavour was Claude E. Shannon who with his famous 1948 article *A Mathematical Theory of Communication* single-handedly created a new discipline: Information Theory! He also revolutionised digital communication and can be seen as one of the main contributors to our modern communication systems like the telephone, the internet etc.

The beauty about information theory is that it is based on probability theory and many results from probability theory seamlessly carry over to information theory. In this chapter, we are going to discuss the bare basics of information theory. These basics are often enough to understand many information-theoretic arguments that researchers make in fields like computer science, psychology and linguistics.

## 7.1 Surprisal and Entropy

Shannon's idea of information is as simple as it is compelling. The amount of *surprisal* of an event $E$ is defined as the inverse probability $1/P(E)$. Intuitively, rare events (where $P(E)$ is small) are more surprising than those occurring with high probability (where $P(E)$ is high). If we are observing a realisation of a random variable, this realisation is surprising if it is unlikely to occur according to the distribution of that random variable. However, if the probability for the realisation is very low, then on average it does not occur very often, meaning that if we sample from the RV repeatedly, we are not surprised very often. We are not surprised when the probability mass of the distribution is concentrated on only a small subset of its support.

On the other hand, we quite often are surprised, if we cannot predict what the outcome of our next draw from the RV might be. We are surprised when the distribution over values of the RV is (close to) uniform. Thus, we are going to be most surprised on average if we are observing realisations of a uniformly distributed RV.

Shannon's idea was that observing RVs that cause a lot of surprises is informative because we cannot predict the outcomes and with each new outcome we have effectively learned something (namely that the $i^{th}$ outcome took on the value that it did). Observing RVs with very concentrated distributions is not very informative under this conception because by just choosing the most probable outcome we can correctly predict most actually observed outcomes. Obviously, if I manage to predict an outcome beforehand, its occurrence is not teaching me anything.

The goal of Shannon was to find a function that captures this intuitive idea. He eventually found it and showed that it is the only function to have properties that encompass the intuition. This function is called the **entropy** of a RV and it is simply the expected **surprisal** value, expressed in bits.

**Definition 7.1 (Surprisal)** *The surprisal (value) of an outcome* $x \in \operatorname{supp}(X)$ *of some RV* $X$ *is defined as* $-\log_2(P(X=x)) = \log_2(\frac{1}{P(X=x)})$.

Notice that we are using the logarithm of base 2 here. This is because surprisal and entropy are standardly measured in bits. Intuitively, the surprisal measures how many bits one needs to encode an observed outcome given that one knows the distribution underlying that outcome. Check this website to get a feeling for surprisal values measured in bits.

**Definition 7.2 (Entropy)** *The entropy* $H(P_X)$ *of a RV* $X$ *with distribution* $P_X$ *is defined as*

$$H(P_X) := \mathbb{E}[-\log_2(P(X=x))] = -\sum_{x \in \operatorname{supp}(X)} P(X=x)\log_2(P(X=x))\,.$$

*For the ease of notation, we often write* $H(X)$ *instead of* $H(P_X)$.

The notational convenience of writing $H(X)$ instead of $H(P_X)$ can be confusing, because entropy is really assigning a (non-negative) real number to a distribution, i.e. $H(X)$ is **not a function** of the random variable $X$ and it is **not a random variable** either! Formally, for any random variable $X$ with distribution $P_X$ over the set $\mathcal{X} = \operatorname{supp}(X)$ (which might be categorical, i.e. $X$ could for instance take on values "blue", "red" and "green"), we consider the surprisal function (in bits) $f(x) := -\log_2(P(X=x))$ mapping elements $x \in \mathcal{X}$ to real numbers $f(x) \in \mathbb{R}$. In that case, the surprisal $f(X)$ is a random variable over the reals and its expected value is well defined and called entropy $H(X) = H(P_X) := \mathbb{E}_X[f(X)]$.

As an example, we consider the categorical random variable $X$ with distribution $P(X = \heartsuit) = P(X = \clubsuit) = 1/4, P(X = \spadesuit) = 1/2$. In that case, $\operatorname{supp}(X) = \{\heartsuit, \clubsuit, \spadesuit\}$ and surprisal values in bits are $f(\heartsuit) = f(\clubsuit) = \log_2(4) = 2, f(\spadesuit) = \log_2(2) = 1$. The entropy is the expected surprisal value, i.e. the individual surprisal valuse weighted with their corresponding probabilities of occurring: $H(X) = \mathbb{E}_X[f(X)] = \frac{1}{4} \cdot 2 + \frac{1}{4} \cdot 2 + \frac{1}{2} \cdot 1 = 3/2$.

The entropy "does not care" about the actual outcomes or labels of a random variable, but only about the distribution! In fact, not even the order of the actual probabilities matter, as we are taking an expected value and the additive terms commute. You can verify that the calculation of $H(X) = 3/2$ in the example above does apply to all random variables $X$ with distribution $(1/2, 1/4, 1/4)$, no matter what the actual outcomes are.

**Exercise 7.3** *Compute the entropy of* $Y \sim$ *Binomial*$(n = 2, p = 1/2)$*.*

The simplest and simultaneously most important example of entropy is given in Figure 7.1 which shows the entropy of the Bernoulli distribution as a function of the parameter $\theta \in [0, 1]$. The entropy function of the Bernoulli is often called the **binary entropy** $h(\theta) := \theta \cdot \log_2(\theta) + (1-\theta)\log_2(1-\theta)$. It measures the information of a binary decision, like a coin flip or an answer to a yes/no-question. The entropy of the Bernoulli attains its maximum of 1 bit when the distribution is uniform, i.e. when both choices are equally probable. The entropy is 0 if and only if the coin is fully biased towards heads or tails. As explained above, the entropy of the distributions $(\theta, 1-\theta)$ and $(1-\theta, \theta)$ is the same and therefore $h(\theta) = h(1-\theta)$ and the graph is symmetric around 1/2.

From the plot is it also easy to see that entropy is never negative. It holds in general that entropy is non-negative, because entropy is defined as expectation of surprisal and surprisal is the negative logarithm of probabilities. Because $\log(x) \leq 0$ for $x \in (0, 1]$, it is clear that $-\log(x) \geq 0$ for $x$ in the same interval. Notice that from here on we drop the subscript and by convention let $\log = \log_2$.

A standard interpretation of the entropy is that it quantifies uncertainty. As we have pointed out before, a uniform distribution means that you are most uncertain and indeed the uniform distribution maximizes the entropy. However, the more choices you have to pick from uniformly, the more uncertain you are going to be. The entropy function also captures this intuition. Notice that if a discrete distribution is uniform, all probabilities are $\frac{1}{|\operatorname{supp}(X)|}$. Clearly, as we increase $|\operatorname{supp}(X)|$, we decrease the probabilities. By decreasing the probabilities, we increase their negative logarithms, and hence their average surprisal. Let us make this intuition more formal.

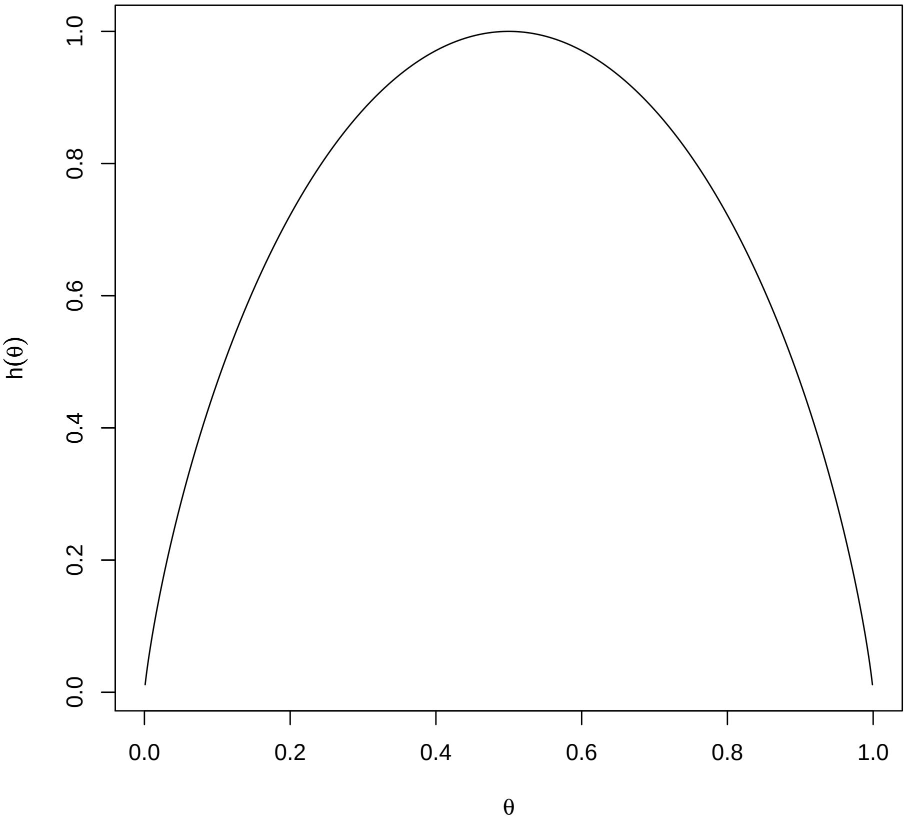


Figure 7.1: Binary entropy function

**Theorem 7.4** *A discrete RV $X$ with uniform distribution and support of size $n$ has entropy $H(X) = \log(n)$.*

**Proof:**

$$H(X) = \sum_{x \in \mathrm{supp}(X)} -\log(P(X = x))P(X = x) \tag{7.1}$$

$$= \sum_{x \in \mathrm{supp}(X)} -\log(\frac{1}{|\,\mathrm{supp}(X)|})P(X = x) \tag{7.2}$$

$$= \sum_{x \in \mathrm{supp}(X)} \log(n)P(X = x) = \log(n)\,. \qquad \Box \tag{7.3}$$

**Exercise 7.5** *You are trying to learn chess and you start by studying where chess grandmasters move their king when it is positioned in one of the middle fields of the board. The king can move to any of the adjoining 8 fields. Since you do not know a thing about chess yet, you assume that each move is equally probable. In this situation, what is the entropy of moving the king?*

One of the first important results in information theory is Shannon's source-coding theorem which states that the entropy $H(X)$ of a random variable $X$ measures how many bits one will need on average to encode an outcome that is generated by the distribution $P_X$. This result applies to the real-world problem of data compression. Assume that $N$ data points are drawn iid from the distribution $P_X$. In that case, the source-coding theorem tells us that on average, we will need $N \cdot H(X)$ bits to store the (optimally compressed) data. For example, let $P_X$ be the *Bernoulli*$(\theta)$ distribution over bits. In the case $\theta = 1/2$, we have $N$ perfectly random bits which cannot be compressed, and hence we need $N \cdot H(X) = N \cdot h(\theta) = N \cdot h(1/2) = N$ bits of storage. For the general case $\theta \neq 1/2$ when the individual bits are biased, the graph of the binary entropy $h(\theta)$ in Figure 7.1 tells us exactly what the compression ratio will be. We will not cover the proof of the source-coding theorem here, but refer to the literature instead.

## 7.2 Conditional Entropy

At the outset of this section we promised you that you could easily transfer results from probability theory to information theory. We will not be able to show any kind of linearity for entropy because it contains log-terms and the logarithm is not linear. We can however find alternative expressions for joint entropy (where the joint entropy is simply the entropy of a joint RV). Before we do so, let us also define the notion of conditional entropy. We have seen in Section 3.3 that $P_{X|Y=y}$ is a valid probability distribution for any $y \in \text{supp}(Y)$ such that $P(Y = y) > 0$. Hence, we can also define its conditional entropy.

**Definition 7.6 (Conditional Entropy)** *For two jointly distributed RVs $X, Y$ and $y \in \text{supp}(Y)$ such that $P(Y = y) > 0$, the conditional entropy of $X$ given that $Y = y$ is defined as*

$$\begin{aligned} H(X|Y = y) &:= \mathbb{E}_X[-\log_2(P(X = x|Y = y))] \\ &= -\sum_{x \in \text{supp}(X)} P(X = x|Y = y) \log_2(P(X = x|Y = y)) \,. \end{aligned}$$

*The conditional entropy of $X$ given $Y$ is defined as*

$$H(X|Y) := \mathbb{E}_Y[H(X|Y)] = \sum_{y \in \mathrm{supp}(Y)} P(Y=y)H(X|Y=y)\,.$$

Intuitively, $H(X|Y)$ is the (average) uncertainty of $X$ after learning $Y$. Intuitively, learning $Y$ (and in fact any information) cannot increase your uncertainty about $X$. Formally, one can prove the following

**Lemma 7.7 (see e.g. Proposition 4 of this script)** *For any two random variables $X, Y$ with joint distribution $P_{XY}$, it holds that $H(X|Y) \leq H(X)$.*

Note however, that this non-increase of uncertainty only holds on average, as illustrated by the following example:

**Example** Consider the binary random variables $X$ and $Y$, with joint distribution

$$\begin{aligned} P(X=0,Y=0) &= \frac{1}{2}, \quad P(X=0,Y=1) = \frac{1}{4} \\ P(X=1,Y=0) &= 0, \quad P(X=1,Y=1) = \frac{1}{4}. \end{aligned}$$

By marginalization, we find that $P(X=0) = \frac{3}{4}$ and $P(X=1) = \frac{1}{4}$, while $P(Y=0) = P(Y=1) = \frac{1}{2}$. This allows us to make the following computations:

$$\begin{aligned} H(X,Y) &= \frac{1}{2}\log 2 + \frac{1}{4}\log 4 + \frac{1}{4}\log 4 = \frac{3}{2} \\ H(X) &= h\left(\frac{1}{4}\right) = h\left(\frac{3}{4}\right) \approx 0.81 \\ H(Y) &= h\left(\frac{1}{2}\right) = 1 \\ H(X|Y) &= P(Y=0)\cdot H(X|Y=0) + P(Y=1)\cdot H(X|Y=1) \\ &= \frac{1}{2}\cdot 0 + \frac{1}{2}\cdot 1 = \frac{1}{2} \\ H(Y|X) &= P(X=0)\cdot H(Y|X=0) + P(X=1)\cdot H(Y|X=1) \\ &= \frac{3}{4}\cdot h\left(\frac{1}{3}\right) + \frac{1}{4}\cdot 0 \approx 0.69 \end{aligned}$$

Note that for this specific distribution, learning the outcome $Y=1$ increases the uncertainty about $X$, $H(X|Y=1) > H(X)$, but on average, we always have $H(X|Y) \leq H(X)$. It is important to remember that Lemma 7.7 only holds on average, not for specific values of $Y$. Note also that in this example, $H(X|Y) \neq H(Y|X)$.

It is not a coincidence that the joint entropy $H(X,Y)$ in the example above is equal to $H(X|Y) + H(Y)$ and $H(Y|X) + H(X)$. One can prove this chain rule in general:

$$\begin{aligned}
H(X,Y) &= \sum_{\substack{x \in \mathrm{supp}(X) \\ y \in \mathrm{supp}(Y)}} -\log(P(X=x,Y=y)) \times P(X=x,Y=y) \\
&= \sum_{\substack{x \in \mathrm{supp}(X) \\ y \in \mathrm{supp}(Y)}} -\log(P(X=x \mid Y=y)) \times P(X=x,Y=y) \\
&\quad - \sum_{y \in \mathrm{supp}(Y)} \log(P(Y=y)) \times \sum_{x \in \mathrm{supp}(X)} P(X=x,Y=y) \\
&= \sum_{y \in \mathrm{supp}(Y)} P(Y=y) \times \sum_{x \in \mathrm{supp}(X)} -\log(P(X=x \mid Y=y)) \times P(X=x \mid Y=y) \\
&\quad - \sum_{y \in \mathrm{supp}(Y)} \log(P(Y=y)) \times P(Y=y) \\
&= H(X|Y) + H(Y)\ .
\end{aligned}$$

**Exercise 7.8** *Prove that* $H(X,Y|Z) = H(X|Z)+H(Y|Z)$ *if* $X \perp Y \mid Z$.

As corollary, we get that $H(X,Y) = H(X) + H(Y)$ for independent random variables $X$ and $Y$. More generally, the entropy of $n$ independent random variables is $H(X_1^n) = \sum_{i=1}^n H(X_i)$.

## 7.3 An Information-Theoretic View on EM

Now that we have seen some information-theoretic concepts, you may be happy to hear that there is an information-theoretic interpretation of EM. This interpretation helps us to get a better intuition for the algorithm. To formulate that interpretation we need one more concept, however.

**Definition 7.9 (Relative Entropy)** *The relative entropy of RVs* $X, Y$ *with distributions* $P_X, P_Y$ *and* $\mathrm{supp}(X) \subseteq \mathrm{supp}(Y)$ *is defined as*

$$D(P_X||P_Y) := \sum_{x \in \mathrm{supp}(X)} P(X=x) \log \frac{P(X=x)}{P(Y=x)}\ .$$

*If* $P(Y=x) = 0$ *for any* $x \in \mathrm{supp}(X)$ *we define* $D(P_X||P_Y) = \infty$. *As with entropy, we often abbreviate* $D(P_X||P_Y)$ *with* $D(X||Y)$.

The relative entropy is commonly known as **Kullback-Leibler (KL)** divergence. It measures the entropy of $X$ as scaled to $Y$. Intuitively, it gives a measure of how "far away" $P_X$ is from $P_Y$. To understand "far away", recall that entropy is a measure of uncertainty. This uncertainty is low if both distributions place most of their mass on the same outcomes. Since $\log(1) = 0$ the relative entropy is 0 if $P_X = P_Y$.

It is worthwhile to point out the difference between relative and conditional entropy. Conditional entropy is the average entropy of $X$ given that you know what value $Y$ takes on. In the case of relative entropy you do not know the value of $Y$, only its distribution.

> **Exercise 7.10** *Show that $D(X, Y||Y) = H(X|Y)$. Furthermore show that $D(X, Y||Y) = H(X)$ if $X \perp Y$.*

Let us start by remembering why we need EM. We have a model that defines a joint distribution over observed ($x$) and latent data ($z$). Such a model generally looks as follows:

(7.4)

$$P(X = x, Z = z \mid \Theta = \theta) = P(X = x \mid Z = z, \Theta = \theta)P(Z = z \mid \Theta = \theta)$$

where we have chosen a factorization that provides a separate term for a distribution over only the latent data.

Recall that the goal of the EM algorithm is to iteratively increase the likelihood through consecutive updates of parameter estimates. These updates are achieved through maximum-likelihood estimation based on expected sufficient statistics. We are now going to show that a) EM computes a lower bound on the marginal log-likelihood of the data in each iteration and b) that this lower bound becomes tight when the expected sufficient statistics are taken with respect to the model posterior. The latter implies that EM performs the optimal update in each iteration.

Let us start by expanding the data log-likelihood and then lower-bounding it.

$$\log(P(X = x \mid \Theta = \theta)) = \log(\sum_y P(X = x, Y = y \mid \Theta = \theta)) \tag{7.5}$$

$$= \log\left(\sum_y Q(Y = y \mid \Phi = \phi)\frac{P(X = x, Y = y \mid \Theta = \theta)}{Q(Y = y \mid \Phi = \phi)}\right) \tag{7.6}$$

$$\geq \sum_y Q(Y = y \mid \Phi = \phi) \log\left(\frac{P(X = x, Y = y \mid \Theta = \theta)}{Q(Y = y \mid \Phi = \phi)}\right) \tag{7.7}$$

Here, we have used Jensen's Inequality to derive the lower bound. Observe that the log is indeed a concave function.

We also have introduced an auxiliary distribution $Q$ over the latent variables with parameters $\phi$. For reasons that we will explain shortly, this distributions is often called the **variational distribution** and its parameters the **variational parameters**. The letter $Q$ is slightly non-standard to denote distributions but we are are following conventions from the field of **variational inference** here.

In the next step, we factorise the model distribution in order to recover a KL divergence term between the variational distribution and the model posterior over latent variables.

$$\sum_y Q(Y = y \mid \Phi = \phi) \log \left( \frac{P(X = x, Y = y \mid \Theta = \theta)}{Q(Y = y \mid \Phi = \phi)} \right) \tag{7.8}$$

$$= \sum_y Q(Y = y \mid \Phi = \phi) \log \left( \frac{P(Y = y \mid X = x, \Theta = \theta) P(X = x \mid \Theta = \theta)}{Q(Y = y \mid \Phi = \phi)} \right) \tag{7.9}$$

$$= \sum_y Q(Y = y \mid \Phi = \phi) \log \left( \frac{P(Y = y \mid X = x, \Theta = \theta)}{Q(Y = y \mid \Phi = \phi)} \right) + \log(P(X = x \mid \Theta = \theta)) \tag{7.10}$$

$$= -D(Q||P) + \log(P(X = x \mid \Theta = \theta)) \tag{7.11}$$

Equation (7.11) gives us two insights. First it quantifies the gap between the lower bound and the actual data likelihood. This gap is equal to the KL divergence between the variational distribution and the model posterior over latent variables. Second, since KL divergence is always positive, the bound only becomes tight when $P = Q$. But this is exactly what is happening in the E-step! The E-step sets $P = Q$ and then computes expectations under that distribution (see Equation (7.7)). Thus, the E-step increases the lower bound on the marginal log-likelihood.

Looking back at Equation (7.7), we also see that the M-step increases the lower bound because it maximises $\mathbb{E}\left[P(X = x, Y = y \mid \Theta = \theta)\right]$. We conclude that both steps are increasing the lower bound on the log-likelihood. We therefore conclude that EM increases the data likelihood in every iteration (or leaves it unchanged at worst).

We will finish with a quick rejoinder on variational inference. EM is a special case of variational inference. Variational inference is any inference procedure which uses an auxiliary distribution $Q$ to compute a lower bound on the likelihood. In the general setting, the auxiliary distribution can be different from the model posterior. This means that the bound never gets tight. However, in models in which the exact posterior is hard (read: impossible) to compute, using a non-tight lower bound instead can be incredibly useful!

The reason this inference procedure is called *variational* is because it is based on the calculus of variations. This works mostly like normal calculus except that standard operations like differentiation are done with respect to functions instead of variables.

## Further Material

At the ILLC, there is a whole course about information theory, currently taught by Christian Schaffner. David MacKay also offers a free book on the subject. Finally, Coursera also offers an online course on information theory.

The information-theoretic formulation of EM was pioneered in this paper. A very recent and intelligible tutorial on variational inference can be found on the archive.