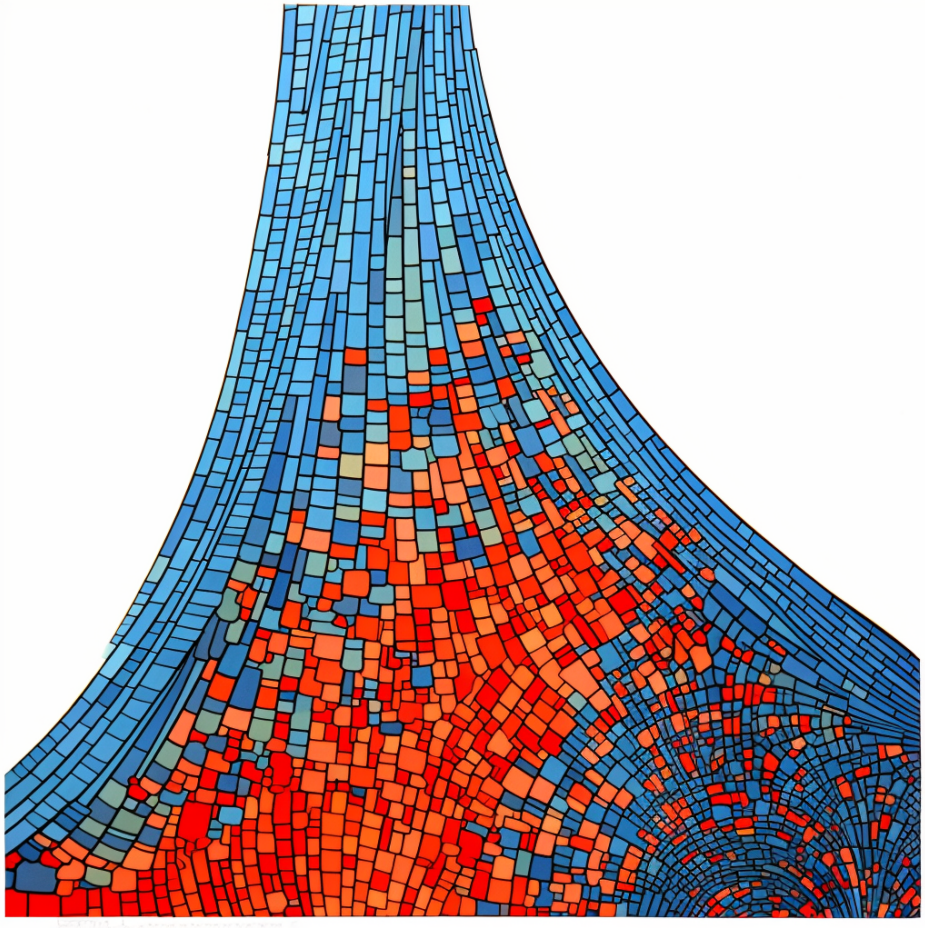
Mattias Villani

Bayesian Learning

The prequel



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Contents

To my students who make it all worthwhile

and a true joy.

Preface

Who is this book for?

This is a book in progress that aims to cover all prerequisites needed for reading my book **Bayesian Learning**. When this prequel is completed, it will contain basic high school algebra, differential calculus, probability and statistical inference, mostly based on likelihood methods.

The book takes the shortest path needed to get to a point where the reading of the Bayesian Learning book is a manageable task. It will therefore skip, or at least pay much less attention to, some concepts that are considered important in Statistics, but which plays only a marginal role in Bayesian statistics, or at least the version of Bayesian statistics covered in my Bayesian Learning book. In particular, there will be only a minimal introduction to frequentist hypothesis testing.

Acknowledgment

I am grateful to Ellinor Fackle-Fornius and Jessica Franzén for letting me use some of their mathematical exercises in this book.

1 Mathematics

This chapter contains a brief review of the basic mathematics used in this book and the Bayesian Learning book, and an introduction to calculus and linear algebra. The treatment is chosen to be light and with a clear forward flow, with rigour sacrificed for ease in presentation. To keep the flow, I will not always qualify the results or concepts to cover all possible special cases and corner cases. No proofs of the presented results are given, and we refer the reader to the book *Real Analysis - a long-form mathematics textbook* by Cummings (2019) for a very accessible long-form presentation of proofs, or any other of the many excellent books used in introductory calculus courses.

The exercises at the end of each section are supposed to help the reader to verify that they have understood and can use the basic concepts, rather than being challenging problems that takes a lot of time and thinking.

1.1 Numbers

We start off on the dry side by defining some number types used in basic mathematics.

Definition. *The* ***natural numbers*** *are* $1, 2, 3, \ldots$.
The set of natural numbers is often denoted by $\mathbb{N} = \{1, 2, 3, \ldots\}$.

Example: The numbers 2.5 and -2 are not natural numbers.

Definition. *An **integer** is*

- *the number zero* 0
- *a natural number* $(1, 2, 3, \ldots)$
- *a negation of a natural number* $-1, -2, -3, \ldots$

The set of integers is often denoted by

$$\mathbb{Z} = \{\ldots, -2, -1, 0, 1, 2, \ldots\}.$$

EXAMPLE: The number -2 is an integer, but 2.5 and $\pi \approx 3.141593$ are not.

Definition. *A **real number** is a number with a potentially infinite number of digits.*
The set of real numbers is typically denoted by $\mathbb{R}$.

EXAMPLE: The number -2 is a real number, and so is $1/3$ and $\pi \approx 3.141593$. The complex number $2 + 3i$ is not a real number, but such numbers are not used in this book.

Sometimes $\mathbb{R}$ is expanded with the symbols ∞ (infinity, something larger than any number) and $-\infty$ (minus infinity, something smaller than any number).

Definition. *A **rational number** is a real number that can be expressed as ratio of two integers* $a = \frac{n}{m}$, *for integer* $n, m \in \mathbb{Z}$.

EXAMPLE: The number 2.5 is a rational number since it can be expressed as a ratio $5/2$ of the two integers 5 and 2. The number π is not a rational number.

Definition. *An **irrational number** is a real number that cannot be expressed as ratio of two integers.*

EXAMPLE: The numbers $\pi \approx 3.141593$ and Euler's number $e \approx 2.71828$ are examples of irrational numbers.

EXERCISES

1. Is $3/2$ an integer?
2. Is the number 1.75 irrational?

1.2 *Basic arithmetics*

The basic arithmetic rules for addition, subtraction, multiplication and division are summarized in Figure 1.2. The reader is no doubt familiar with these rules, but in case of doubt, do a quick check of the exercises.

Basic arithmetics

$$a + b = b + a \qquad a \cdot b = b \cdot a$$
$$a - (-b) = a + b \qquad -a(b + c) = -ab - bc$$
$$a(b + c) = ac + ac \qquad a\left(\frac{b}{c}\right) = \frac{ab}{c}$$
$$\frac{a + b}{c} = \frac{a}{c} + \frac{b}{c} \qquad \frac{a}{b} + \frac{c}{d} = \frac{ad + bc}{bd}$$
$$\frac{\frac{a}{b}}{c} = \frac{a}{bc} \qquad \frac{\frac{a}{b}}{\frac{c}{d}} = \frac{ad}{bc}$$
$$(a + b)^2 = a^2 + 2ab + b^2 \qquad (a + b)(a - b) = a^2 - b^2$$

EXERCISES

1. Simplify the expression $\frac{1}{2} + \frac{3}{4}$
2. Simplify the expression $\frac{1}{3} + \frac{3}{4}$
3. Simplify $ac - a(b + c)$
4. Simplify $a\left(\frac{a}{b}\right)$
5. Calculate $\frac{2}{4} \cdot \frac{3}{2}$
6. Calculate $2 \cdot 4 + \frac{15}{3 \cdot 5}$
7. Simplify $\frac{\frac{5}{4}}{3}$
8. Factorize $a^2 - b^2 + a + b$, where factorize means to write the expression as a product of two or more expressions.
9. Simplify $(a + b)^2 - (a - b)^2$

1.3 *Equations and inequalities*

An **equation** is a mathematical formula that equates two expressions. For example, Einstein's famous formula $E = mc^2$ equates the energy of particle E with its mass m times the speed of light c squared. The equation often involves an unknown variable x, for example $x^2 - 2x = 0$, and we try to **solve the equation** for x; that is, we search for the value of x that satisfies the equation. Sometimes there

equation

solve the equation

is no such solution, in other cases there is a single solution or even many solutions.

Linear equations $a \cdot x + b = 0$ with constants a and b are particularly easy to solve. We are allowed to manipulate the equation, for example by addition, subtraction, multiplication and division, provided that we perform the same operation on both sides of the equation. For example, when solving for x in the linear equation $-3 \cdot x + 2 = 0$, we can subtract 2 from both sides to obtain

$$-3 \cdot x + 2 - 2 = 0 - 2 \quad \Longleftrightarrow \quad -3 \cdot x = -2$$

and then divide by -3 on both sides to isolate x alone on the left hand side of the equation

$$\frac{-3 \cdot x}{-3} = \frac{-2}{-3} \quad \Longleftrightarrow \quad x = \frac{2}{3}.$$

We can verify that this is a correct solution by inserting $x = 6$ in the equation and see that $-3 \cdot (2/3) + 2$ is indeed zero.

Sometimes the relationship between variables is not an equality, but an **inequality**. For example, if x is my age, then sadly $x > 50$, meaning that I am more than 50 years old. A couple of years ago, when I had not turned 50, I would have written $x < 50$. The inequality $x > 50$ is a **strict inequality**, meaning that the statement $x > 50$ is only true if x is larger than 50, but not if $x = 50$ exactly. If we want to include also this case then we write $x \geq 50$ which is now true for x larger than 50, but also for $x = 50$.

inequality

strict inequality

Inequalities can be manipulated in a similar fashion as equalities by addition, subtraction, multiplication and division. However, with inequalities we need to be careful with multiplication and division, which may change the direction of the inequality. For example, the inequality $x > 50$ retains its direction (larger than) when the number 5 is subtracted from both sides:

$$x > 50 \quad \Longleftrightarrow \quad x - 5 > 50 - 5,$$

or when both sides are multiplied by a positive number

$$x > 50 \quad \Longleftrightarrow \quad x \cdot 5 > 50 \cdot 5.$$

But when both sides are multiplied or divided by a *negative* number, the inequality is *reversed*

$$x > 50 \quad \Longleftrightarrow \quad x \cdot (-5) < 50 \cdot (-5).$$

There is of course nothing strange about this: for example, $5 < 10$ while $-5 > -10$.

EXERCISES

Equations and inequalities

1. Solve the equation $3x - 2 = 0$ for x.
2. Solve the equation $4x + 3 = 0.5x$ for x.
3. Solve the equation $2y + 3x = 4$ for y.
4. Rewrite the inequality $2 + x \geq 4$ so that only x is on the left hand side.
5. Rewrite the inequality $1 - x > -6$ so that only x is on the left hand side.

1.4 Sums and products

The **summation symbol** $\sum$ is used to denote the sum (addition) of a sequence of numbers or other mathematical object like functions; the symbol itself is supposed to look like the letter s as in word sum. In the sum $\sum_{k=1}^{n} k$, the **subscript** $k = 1$ below the summation symbol indicates that the sum starts at $k = 1$, and the **superscript** n above the summation symbol indicates that the sum ends when $k = n$. For example, the sum of the first 4 natural numbers is denoted as $\sum_{k=1}^{4} k = 1 + 2 + 3 + 4 = 10$, or a bit more generally, the sum of the first n natural numbers is

summation symbol

subscript

superscript

$$\sum_{k=1}^{n} k = 1 + 2 + 3 + \ldots + n,$$

where the three dots denotes that there are more terms in the sum, but their pattern is clear. The terms in the sum can be functions of the index variable k, for example the sum of squares $\sum_{k=1}^{n} k^2 = 1^2 + 2^2 + 3^2 + \ldots + n^2$. The sum of squares of all even natural numbers smaller than 10, i.e. $2^2 + 4^2 + 6^2 + 8^2$, can be expressed as $\sum_{k=1}^{4} (2k)^2$.

The **index variable** k in the sum $\sum_{k=1}^{n} k$ is just a dummy variable and we can equally well use any other letter or symbol. So, $\sum_{k=1}^{n} k$ is exactly the same sum as $\sum_{i=1}^{n} i$. The summation index k does not need to start from 1, for example the sum $\sum_{k=3}^{5} k = 3 + 4 + 5$ is valid.

index variable

In statistics we often sum data points $x_1, x_2, \ldots, x_n$ where x_i is the value of the ith observation in a sample of n observations. The sample mean is the sum of all data points divided by the sample size

$$\bar{x} = \frac{x_1 + x_2 + \ldots + x_n}{n} = \frac{\sum_{i=1}^{n} x_i}{n}.$$

The sample standard deviation measures the variability or spread in the data as the average squared deviation from the sample mean

$$s^2 = \frac{(x_1 - \bar{x})^2 + (x_2 - \bar{x})^2 + \ldots + (x_n - \bar{x})^2}{n} = \frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n}.$$

It is common to divide by $n-1$ instead of n in the sample standard deviation, for reasons that will be explained later in the book. The point here is the both sample mean and sample standard deviation involves sums, as do many other statistical concepts, so it is important to get used to the summation symbol. When the range of the summation index (the subscript and superscripts) is obvious from the context, it is sometimes skipped and the sample mean can for example be written as $\frac{\sum x_i}{n}$.

Another common symbol is the **product symbol** $\prod$, which is used to denote the multiplication of a sequence of numbers or other mathematical objects. The product of the first n natural numbers is denoted as $\prod_{k=1}^{n} k = 1 \cdot 2 \ldots \cdot n$, we just as for the summation symbol we have a dummy index variable k that starts from the value in the subscript, in this example 1, up to the value in the superscript, in this case n. The product of descending natural numbers $n \cdot (n-1) \cdots 2 \cdot 1$ has its own name, the **factorial**, and is denoted by $n!$. Using the product symbol we can write $n! = \prod_{k=1}^{n} k$. The product symbol appears frequently in probability and statistics since the joint probability of several independent events is the product of the individual event's probabilities.

product symbol

EXERCISES

Sums and products

1. Calculate $\sum_{k=1}^{4} k$
2. Calculate $\sum_{i=1}^{4} k$
3. Calculate $\sum_{y=1}^{3} y^2$
4. Calculate $\left(\sum_{y=1}^{3} y\right)^2$
5. Calculate $\prod_{k=1}^{4} k$
6. Calculate $\prod_{i=1}^{4} k$
7. Calculate $\prod_{i=1}^{3} i^2$
8. Calculate $\left(\prod_{i=1}^{3} i\right)^2$

1.5 *Combinatorics*

The field of mathematics called *combinatorics* is the **mathematics of counting**, for example counting the number of ways that elements can be selected from a collection of objects.

A **set** is an unordered collection of distinct objects referred to as the *elements* of the set. The elements can be anything, for example numbers, colored balls, or people. We often write a set using curly

set

braces, for example $S = \{1, 2, 3\}$ is a set with three integers or a set of three colored balls $B = \{\bullet, \bullet, \bullet\}$. The unordered aspect in the definition means that the sets $\{1, 2, 3\}$ and $\{2, 1, 3\}$ are considered the same set, the order of the elements does not matter. We often determine the elements of a set by some condition, for example the set of all even natural numbers, where evenness is the condition. This set can be written as

$$E = \{x \in \mathbb{N} : x \text{ is even}\} = \{2, 4, 6, \ldots\},$$

where $\mathbb{N}$ is the set of natural numbers and the colon : is to be read as 'such that'. The above set E is therefore read as 'all x in the set of natural numbers such that x is even'. Note also that sets can have an infinite number of elements, for example the set of all even natural numbers is clearly infinite.

If we have a set of three balls with different colors – orange, blue and green – and we want to select two of them, how many different ways can this be done? The answer depends on whether the selection is done

- with or without *replacement*, and
- if the *order* in which the balls are drawn matters.

Selection with replacement

Selection with replacement means that each selected element is returned to the set after the draw, so that it can be selected again.

Selection without replacement

Selection without replacement is when the selected element is not returned to the set after the draw; here the same element cannot be selected again.

With respect to order

With respect to order means that the order in which the elements are drawn matters, so that for example the two draws $(\bullet, \bullet)$ and $(\bullet, \bullet)$ are considered different events. If the order does not matter, then these two draws are considered the same event 'one orange and one green ball'. A selection where the order does not matter is called a **combination**, while a selection where the order matters is called a **permutation**.

combination

permutation

We will introduce the concepts of selection with and without replacement, and the order in which the elements are drawn, by considering a simple example with the selection of $k = 2$ balls from a set of $n = 3$ balls of different colors. The general case with the selection of k elements from a set of n elements is given at the end of this section.

Example: Selection with replacement. Consider first the case where two balls are randomly drawn from an urn with three colored balls, one of each color. Assume first that the order in which the balls is considered important. On the first draw, we have three possible

outcomes: ●, ● or ●; this is illustrated by the bottom fork in the upper half of Figure 1.1, where each of the three possible branches lead to one of the colors. On the second draw we have again three possible outcomes, since the selected ball is returned to the urn after the draw; this is illustrated by the three top forks in Figure 1.1, each originating from the selected color in the first draw. Hence, there are $3 \cdot 3 = 9$ different ways that two balls can be drawn from the urn, as listed to the right in top part of Figure 1.1.

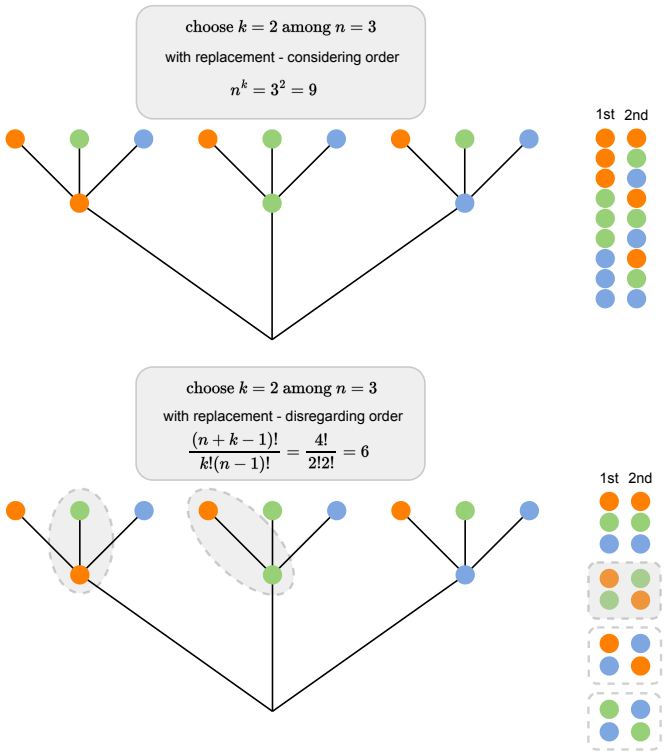

Figure 1.1: Illustrating the number of ways that $k = 2$ balls can be chosen *with replacement* from an urn with $n = 3$ balls with different colors. With replacement means that the selected ball from the first draw is returned to the urn after the draw. The top graph shows the case where the order in which the balls are drawn matters. The nine different combinations are listed to the right. The bottom graph shows the case where the order is disregarded. Selecting one green and one orange ball is here considered the same event, regardless of which of the two colors was drawn first; this is illustrated by the gray dashed areas for the case with one green and one orange ball in the two draws; there is only six different outcomes, three for the cases where the same color is drawn in both attempts, plus another three outcomes with mixed colors on the drawn balls.

Suppose now that the order in which the balls are drawn does not matter, so that for example both the outcomes (●, ●) and (●, ●) are counted as the same event 'one orange and one blue ball'. The number of ways that two elements out of a total of three elements can be chosen is then $3 + 3 = 6$ since there are three outcomes where the same color is drawn in both attempts, plus another three outcomes where the two drawn balls have different colors. This is illustrated in the bottom part of Figure 1.1 where the two draw sequences (●, ●) and (●, ●) are group together as one event.

EXAMPLE: SELECTION WITHOUT REPLACEMENT. Consider now the case without replacement. The top graph in Figure 1.2 illustrates the case where the order in which the balls are drawn matters. As before, the first draw has three possible outcomes, but the second

draw has now only two possible outcomes, since the selected ball is not returned to the urn after the draw. This gives $3 \cdot 2 = 6$ different combinations, as listed to the right in the top part of Figure 1.2.

Finally, the case without replacement but where the order in which the balls are drawn does not matter; this case is illustrated in the bottom graph of Figure 1.2. Here there are only three different outcomes, as listed to the right in the bottom part of Figure 1.2.

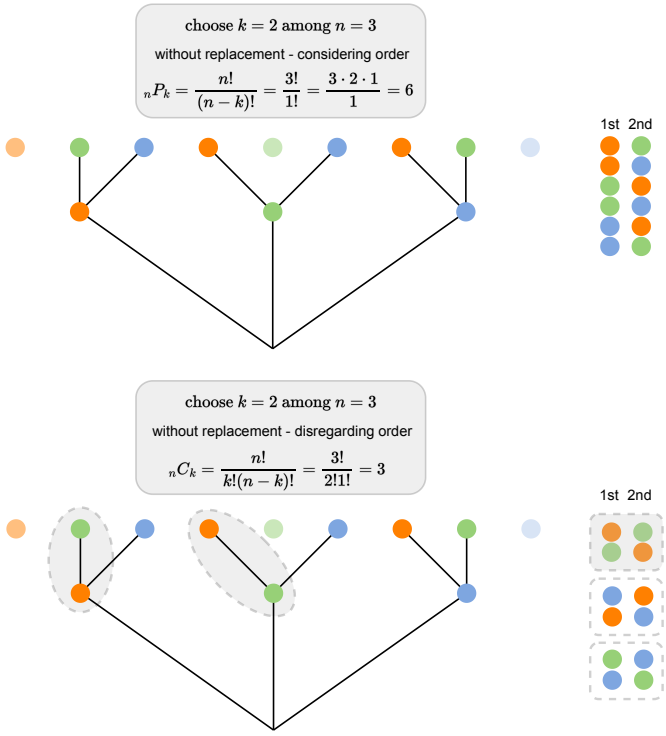

Figure 1.2: Illustrating the number of ways that $k = 2$ balls can be chosen *without replacement* from an urn with $n = 3$ balls with different colors. Without replacement means that the selected ball from the first draw is not returned to the urn after the draw. The top graph shows the case where the order of the element matters; i.e. selecting an orange ball on the first draw and green on the second draw is considered a different case than selecting green ball first followed by an orange. This give six different combinations. In the bottom graph, the order is disregarded. Selecting one green and one orange ball is considered the same event, regardless of which of the two colors was drawn first; this is illustrated by the gray dashed areas for the case with one green and one orange ball in the two draws. Here there is only three different outcomes.

Table 1.3 summarizes the number of ways that k elements can be chosen from a set of n elements, with and without replacement, and with and without respecting the order in which the elements are drawn. This generalizes the examples above to the case with n balls, each with a different color, with k draws from the urn.

The top left cell with replacement and with respect to order is the easiest to understand, since there are n possible outcomes for each of the k draws, giving $n \cdot n \cdots n = n^k$ different ways that k elements can be chosen from n elements.

The case without replacement and respecting order (top right of Table 1.3) is also fairly easy to grasp, since there are n possible outcomes for the first draw, but only $n - 1$ for the second draw, $n - 2$ for the third draw and so on until the kth and last draw where there are $n - k + 1$ remaining balls to choose from. Hence the total number

of ways is

$$n(n-1)\cdots(n-k+1) = \frac{n!}{(n-k)!},$$

where the symbol $n!$ denotes the **factorial** of the positive integer n defined as

factorial

$$n! = n(n-1)\cdots 2\cdot 1, \tag{1.1}$$

and we also let $0! = 1$ by definition.

The case without replacement and without respecting order (bottom right of Table 1.3) is a bit more tricky, but can be understood by considering the number of ways that k elements can be chosen from n elements, and then dividing by the number of ways that the k selected elements can be internally ordered. With k selected elements, there are $k! = k\cdot(k-1)\cdots 2\cdots 1$ ways that they can be ordered. For example, let us add also a yellow ball so that there are now $n = 4$ different colors, and we select $k = 3$ of them without replacement. Given a selection of $k = 3$ colors, there is $3\cdot 2\cdot 1 = 6$ ways that we can obtain the three colors. The total number of ways that we can select $k = 3$ balls from $n = 4$ colors is therefore

$$\frac{4\cdot 3\cdot 2\cdot 1}{3\cdot 2\cdot 1} = 4.$$

This particular example can be solved more easily by considering that each outcome with $k = 3$ drawn elements from $n = 4$ can equally well be represented by the one color was *not* drawn, and there are 4 different colors to choose from. The number of ways k elements can be drawn without replacement from n elements, without regard for the order in which the elements are drawn number, has its own symbol, the **binomial coefficient**:

binomial coefficient

$$\binom{n}{k} = \frac{n!}{k!(n-k)!} \tag{1.2}$$

The final case in the lower left cell of Table 1.3 is the case with replacement and disregarding order. This will not be used in this book, but can be argued to be have $\binom{n+k-1}{k}$ possible outcomes.

How many ways can we choose k elements from n elements?		
	with replacement	without replacement
respecting order	n^k	$\frac{n!}{(n-k)!} = n(n-1)\cdots(n-k+1)$
disregarding order	$\binom{n+k-1}{k} = \frac{(n+k-1)!}{k!(n-1)!}$	$\binom{n}{k} = \frac{n!}{k!(n-k)!}$

Figure 1.3: The combinatorics of selecting elements.

EXERCISES

Combinatorics

1. How many ways can you select 3 balls from an urn with 4 different colored balls, with replacement and with respect to the order in which the balls are drawn?
2. You have four friends, but only two extra tickets for the cinema on Friday. How many ways can you select two friends to join you at the cinema?

1.6 Exponential numbers

Here is the definition of a power of a number.

Definition. *The **nth power** of a number b is defined as*

$$b^n = \underbrace{b \cdot b \cdots b}_{n \text{ times}}$$

*A number of the form b^n is also called an **exponential number** with **base** b and **exponent** n.*

The term **exponentiation** refers to the operation of computing powers. exponentiation

The rules for exponential numbers in Figure 1.6 should be known by heart, but are also rather easy to recreate yourself from the definition of an exponential number. For example

$$a^n a^m = \underbrace{a \cdot a \cdots a}_{n \text{ times}} \cdot \underbrace{a \cdot a \cdots a}_{m \text{ times}} = \underbrace{a \cdot a \cdots a}_{n+m \text{ times}} = a^{n+m}.$$

Note that either the base or the exponent must be the same for the rules to be applicable; for example, $a^n a^m = a^{n+m}$ (same base) and $a^n b^n = (ab)^n$ (same exponent), but the product of a^n and b^m (different base and exponent) is $a^n b^m$ and cannot be simplified.

Rules for exponents

$$a^n a^m = a^{n+m} \qquad a^n b^n = (ab)^n$$
$$(a^n)^m = a^{nm} \qquad a^0 = 1$$
$$\frac{a^n}{a^m} = a^{n-m} \qquad \left(\frac{a}{b}\right)^n = \frac{a^n}{b^n}$$
$$a^{-n} = \frac{1}{a^n} \qquad \sqrt{a} = a^{1/2}$$

EXERCISES

Exponentiation

1. Calculate $(-2)^3$
2. Calculate 0.1^2
3. Simplify $3^2 \cdot 3^5$
4. Simplify $(2^4)^2$
5. Simplify $\frac{a^3}{a^2}$
6. Simplify $\frac{a^3}{a^5}$
7. Simplify $\frac{6^3}{2^3}$
8. Simplify $\frac{6 \cdot 10^{-4}}{3 \cdot 10^{-6}}$
9. Simplify $a \cdot \frac{b^2}{a^3}$

1.7 *Logarithms*

A **logarithm** is the inverse to an exponential number, in a way that we will soon explain. Let us work up to the definition of a logarithm by some concrete examples.

logarithm

- The logarithm with base 10 (the 10-logarithm) of the number 1000 is 3, because 1000 is the base 10 raised to the 3

  $$10^3 = 1000$$

  We write the 10-logarithm as $\log_{10}$, so $\log_{10}(1000) = 3$.

- The logarithm with base 2 (the 2-logarithm) of the number 256 is 8, because 256 is the base 2 to the 8th power

  $$2^8 = 256$$

  We write the 2-logarithm as $\log_2$, so $\log_2(256) = 8$.

- The **natural logarithm** of the number 256 is approximately 5.54518, because

  $$e^{5.54518} \approx 256$$

  where $e \approx 2.71828$ is Euler's number, which is therefore the base for the natural logarithm. We write the natural logarithm as $\log_e$ or ln, so $\ln(256) \approx 5.54518$.

natural logarithm

The pattern above gives the general definition of a logarithm

Definition. *The **logarithm with base** b of a positive number x is the number a such that*

$$x = b^a$$

We write $a = \log_b(x)$.

A natural logarithm with the complicated number e as base may not seem like the most natural way to define a logarithm, but it will be the main logarithm used in this book; one reason for this choice is that derivation and integration becomes particularly easy with this base, as we will see in Sections Differentiation and Integration. When we write log without an explicit base, we mean the *natural* logarithm. It is also common to shorten the word *logarithm* to just *log*, and to say, for example, 'the log of 2 is approximately 0.693'.

The rules for calculating with logarithms are given in Figure 1.4. The figure uses the natural logarithm with base e, but similar rules hold for other bases; for example the rule for the logarithm of a product for a general base b is

$$\log_b(x \cdot y) = \log_b(x) + \log_b(y),$$

assuming that x and y are positive and that $b \neq 1$. This is a very important and useful property of logarithms: **a logarithm turns a product into a sum** (of logs). To see that this is indeed the case, let $x = b^n$ and $y = b^m$ be exponential numbers with the same base b. The product rule for exponential numbers then says that $x \cdot y = b^n \cdot b^m = b^{n+m}$. Now, from the defintion of the logarithm we have $n = \log_b(x)$, $m = \log_b(y)$ and $\log_b(x \cdot y) = \log_b(b^{n+m}) = n + m = \log_b(x) + \log_b(y)$.

Rules for logarithms

$\log(e) = 1$	$\log(1) = 0$
$\log(x \cdot y) = \log x + \log y$	$\log\left(\frac{x}{y}\right) = \log x - \log y$
$\log x^y = y \log x$	$\log e^y = y \log e = y$

Figure 1.4: Rules for the natural logarithm for positive real numbers x and y. The symbol log is used for the natural logarithm with base e. The rules are similar for other bases.

We can repeat this product rule for logarithms twice to show that the log of a product of *three* positive numbers is

$$\log(x \cdot (y \cdot z)) = \log(x) + \log(y \cdot z) = \log(x) + \log(y) + \log(z).$$

Similarly, for any number of factors in the product:

$$\log(x_1 \cdot x_2 \cdots x_n) = \log(x_1) + \log(x_2) + \ldots + \log(x_n),$$

where $x_1, x_2, \ldots, x_n$ are positive real numbers. Let us take the opportunity to write this last equation using the summation and product symbols from Section Sums and products:

$$\log\left(\prod_{i=1}^{n} x_i\right) = \sum_{i=1}^{n} \log(x_i).$$

This property of the log, and the notation with sums and product symbols is used a lot in statistics, for example when working with the so called log-likelihood function introduced in Section Maximum likelihood; do not gloss over this, it will come back many times.

The other important rule which holds for any base (and is really just a special case of the previous rule for the log of a product) is the logarithm of an exponential number

$$\log_b(x^y) = y \log_b(x).$$

This shows that logs 'pull down exponents'. In particular, when the logarithm is defined in the same base as the exponential number, we have $\log_b(b^y) = y \log_b(b) = y \cdot 1 = y$. This is very useful when we try to solve equations where the unknown x appears as an exponent, for example $a^x = c$. Taking logs on both sides gives $x \log(a) = \log(c)$ (note how x is no longer a power, but a simple multiplicative factor), and dividing both sides by $\log(a)$ gives the solution $x = \log(c)/\log(a)$.

EXERCISES

Exponentials and logarithms

1. Simplify $e^{\ln(3)}$
2. Simplify $\ln(e^4 e^{-2})$
3. Simplify $\frac{6e^{3x}}{2e^x}$
4. Simplify $\log_2(8) + \log_3(27)$
5. Solve $3^{2x-1} = 27$
6. Solve $2 - \ln(3x - 2) = 10$
7. Solve $\ln(x) - \ln(x - 2) = 2$
8. Solve $y = \ln\left(\frac{x}{1-x}\right)$ for x

1.8 *Functions*

Functions

A *function* can be loosely thought of as something that takes an input x, does something to it, and returns an output y; see Figure 1.5. The

input is often called the **argument** of the function, and the output is also called the **function value**.

Formally, a **function** $f(x)$ maps each element x in a set $\mathcal{X}$ to exactly one element y in another set $\mathcal{Y}$; we write $y = f(x)$ when we want to explicitly show the output of the function. The set $\mathcal{X}$ is called the **domain** of the function and the set $\mathcal{Y}$ is called the **codomain** of the function. Not all values in the codomain will necessarily be attainable from any x in the domain $\mathcal{X}$, and the set of elements that are mapped to at least one $x \in \mathcal{X}$ is called the **range** or the **image** of the function $f(x)$; Figure 1.6 illustrates these concepts. Both the domain and the codomain will in most cases here be a real interval $[a, b] \in \mathbb{R}$; the interval could be open (a, b) or half-open $[a, b)$, and the boundaries can sometimes be ∞ or $-\infty$, for example $[0, \infty)$ or $(-\infty, \infty)$.

argument

function value

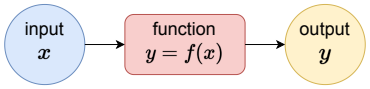

Figure 1.5: Illustration of a function.

function

domain

codomain

range

image

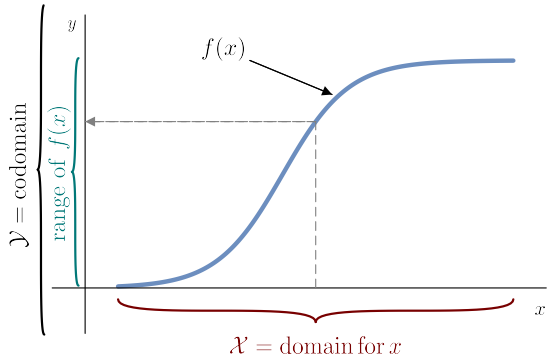

Figure 1.6: A function with its domain, codomain and range.

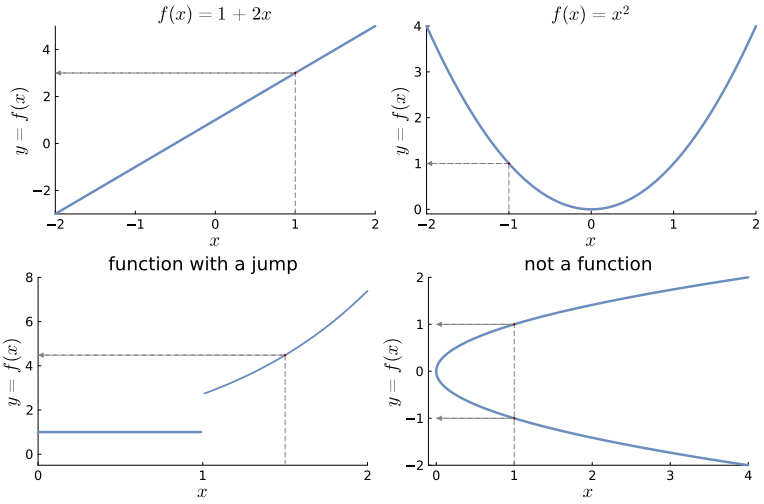

Figure 1.7: Some example functions and a non-function.

Figure 1.7 illustrates some functions. The linear function $f(x) =$

$1 + 2x$ and the quadratic function $f(x) = x^2$ in the top row are smooth without jumps. The bottom left graph shows a function that is smooth over most x-values, but with an abrupt jump at $x = 1$. The bottom right graph in Figure 1.7 shows an example of a relation that is not a function, since the input $x = 1$ is mapped to two different outputs $y = -1$ and $y = 1$, so it violates the requirement that each input is mapped to *exactly one* output. Note that the top right graph of the square function $f(x) = x^2$ *is* a function, even though both inputs $x = -1$ and $x = 1$ are mapped into the same output $f(-1) = f(1) = 1$; the requirement of a function is only that each x should be mapped to exactly one output; an output value is allowed to correspond to multiple input values.

Section Exponential numbers introduced the exponential number, i.e. powers with a certain base b, for example the natural exponential with base $e \approx 2.71828$, the Euler number. The **exponential function** $f(x) = e^x$ is a function that maps each real number $x \in \mathbb{R}$ to the exponential number $y = e^x$. For example, when we insert the input $x = 0$ in the exponential function we get $f(0) = e^0 = 1$, and when we plug in the input $x = 1$ we get $f(1) = e^1 = e$. This function is so important that it gets its own definition box:

exponential function

Definition. *The (natural)* ***exponential function***

$$f(x) = e^x$$

maps real numbers $x \in \mathbb{R}$ to the exponential number e^x with base e.

Figure 1.7 plots the exponential function $f(x) = e^x$ for all inputs in the interval $(-2, 2)$, and marks out the function evaluation at $x = 1$.

The exponential function $f(x) = e^x$ is an example of a (strictly) *monotonically increasing function* since

$$x_1 < x_2 \implies f(x_1) < f(x_2),$$

for all pairs of inputs x_1 and x_2 in the domain; that is, increasing the input gives a larger output. A (strictly) *monotonically decreasing function* instead satisfies

$$x_1 < x_2 \implies f(x_1) > f(x_2),$$

meaning that a larger input leads to a smaller output. A function is a **monotone function** if is either monotonically increasing or monotonically decreasing throughout its domain.

monotone function

The exponential function is sometimes confused with the **power function**:

power function

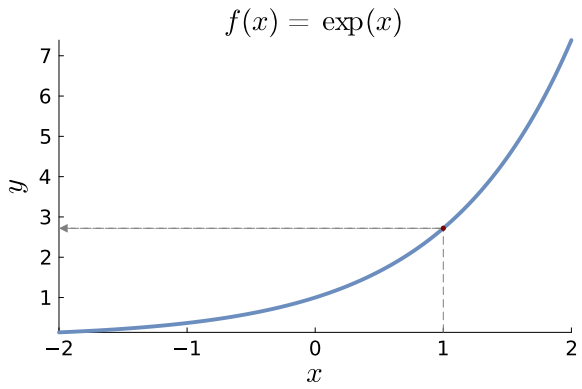

Figure 1.8: The exponential function $f(x) = \exp(x)$ plotted over the interval $x \in (-2, 2)$.

Definition. *The **power function***

$$f(x) = x^p$$

maps real numbers $x \in \mathbb{R}$ to the exponential number x^p with base x and exponent, or power, $p \in \mathbb{R}$.

Note the difference in where the x is located in

- the exponential function $f(x) = b^x$, for some base b and
- the power function $f(x) = x^p$, for some exponent p.

Figure 1.9 plots some power functions for different powers p. The case $p = 1/2$ is the power function $f(x) = x^{1/2}$, which is the square root function $f(x) = \sqrt{x}$.

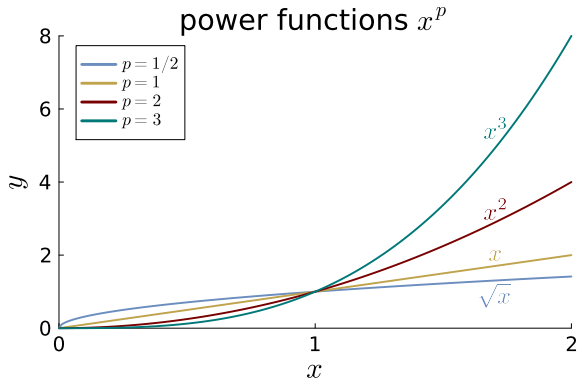

Figure 1.9: The power function $f(x) = x^p$ plotted over the interval $x \in (0, 2)$ for different powers.

A **polynomial function** is weighted sum of power functions with different powers. Such a weighted sum is more often a called a *linear combination*. Here is the definition of the polynomial function.

polynomial function

Definition. *A **polynomial function** of degree p is a linear combination of power functions*

$$f(x) = a_0 + a_1 \cdot x + a_2 \cdot x^2 + \ldots + a_p \cdot x^p,$$

*where $a_0, a_1, \ldots, a_p$ are real-valued **polynomial coefficients**.*

The degree of the polynomial is the highest power p in the function. Some of the polynomial coefficients can be zero so that, for example, the function $f(x) = 1 + 2x^2 - 3x^4$ is a polynomial of degree 4 even though it lacks the first and third powers. Figure 1.10 plots some polynomial functions with different degrees and coefficients.

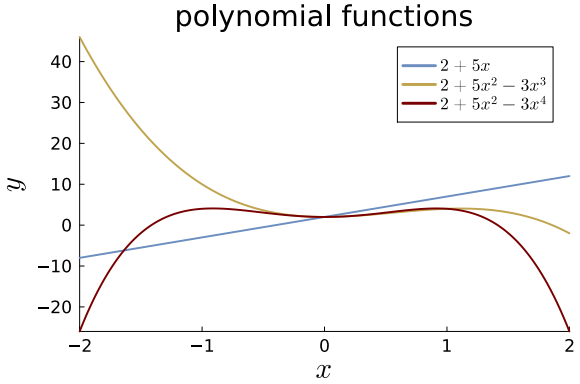

Figure 1.10: Some polynomial functions.

EXERCISES

Functions

1. Compute $f(2) - f(-1)$ when $f(x) = x^2 + 3^x$
2. Sketch the function $g(x) = 3x^3$ over the interval $[-1, 1]$ on a piece of paper.

1.9 *Composite functions*

It is common to combine two functions so that the output z from one function $z = h(x)$ is used as an *input* in the other function $y = g(z)$. Figure 1.11 gives a flow chart presentation of this **function composition** idea. If you have some experience with computer programming, this idea is probably not new to you; computer code is often written in a *modular* way with one function called from within another function. The end result from function composition is a new function that maps the original input x to the final output y. The mathematical

function composition

formulation of the flow chart in Figure 1.11 is

$$y = g(h(x))$$

where the function h is called the **inner function** and g is called the **outer function**. Since $g(h(x))$ is a new function we may sometimes introduce a new symbol for it, for example $f(x) = g(h(x))$. The composition of the functions g and h is also denoted by $g \circ h$, or $(g \circ h)(x)$, but we will not use that notation in this book.

inner function

outer function

Figure 1.11: Illustration of a composite function $y = g(h(x))$ where an input x is fed to the inner funtion $h(x)$ to produce the output $z = h(x)$, which is then fed to the second function that returns the final output $y = g(z)$.

EXAMPLE: Let $h(x) = x^2$ and $g(x) = \ln(x)$. Figure 1.12 plots these functions and the composition $f(x) = g(h(x))$.

EXAMPLE: Let $h(x) = -x^2$ and $g(z) = \frac{1}{\sqrt{2\pi}} \exp\left(\frac{1}{2}z\right)$. The composition of these two function, with h as the inner function,

$$f(x) = g(h(x)) = \frac{1}{\sqrt{2\pi}} \exp\Big(-\frac{1}{2}x^2\Big), \tag{1.3}$$

is the bell-shaped Gaussian probability distribution that we will meet many times later in this book.

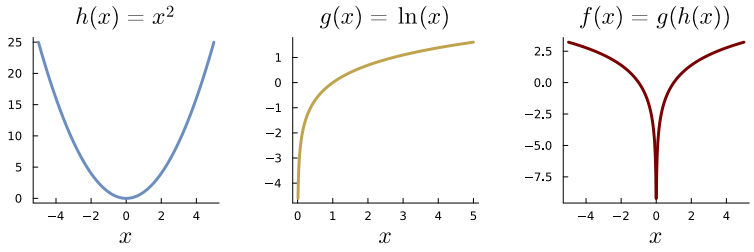

Figure 1.12: Illustration of a composite function $y = g(h(x))$, with inner funtion $h(x) = x^2$ and outer function $g(x) = \ln(x)$.

We have carefully used different variable names (x and z) in the inner and outer functions above. However, since variable names in functions are just dummy variables without real meaning, we can use the same name for the input variable in both the inner and outer function; it is therefore perfectly fine to talk about the composition $g(h(x))$ of the two functions $g(x)$ and $h(x)$. We can skip the dummy variable x completely, and just say the composition of the functions g and h, as long as it is clear which function is the inner one of the two.

We cannot wildy compose just any two functions. The outer function g must be able to accept the kind of output produced by the inner function h. In mathematical terminology, the range of the inner function h must be a subset of the domain of the outer function g. For example, the linear function $h(x) = 1 + 2x$ for $x \in \mathbb{R}$ cannot be composed with the logarithm function $g(x) = \log(x)$, since the inner function $h(x)$ gives negative output for all $x < -1/2$ and the outer logarithm function is not defined for negative inputs.

EXERCISES

Functions

1. Let $h(x) = x^2$ and $g(x) = \ln(x)$. Write code for these mathematical functions as as separate functions in your favorite programming language. Use these two functions in a third function that computes the composition $f(x) = g(h(x))$. Use the code to plot the inner, outer and composed function.

1.10 *Inverse function*

Recall that the range of a function is the set of all possible values that the function can output, i.e. the set of all y such that $y = f(x)$ for some input $x \in \mathcal{X}$. The range can be a subset of the codomain $\mathcal{Y}$. A function is said to be **bijective**, or **one-to-one and onto**, if it

bijective

one-to-one and onto

- maps distinct x to distinct y (one-to-one), and
- its range is the whole codomain (onto)

The exponential function in the left graph of Figure 1.13 is bijective with domain $\mathcal{X} = (-\infty, \infty)$ and codomain $\mathcal{Y} = (0, \infty)$. The quadratic function in the top right graph of Figure 1.7 is not one-to-one since distinct x, for example $x = -1$ and $x = 1$, maps into the same $y = 1$.

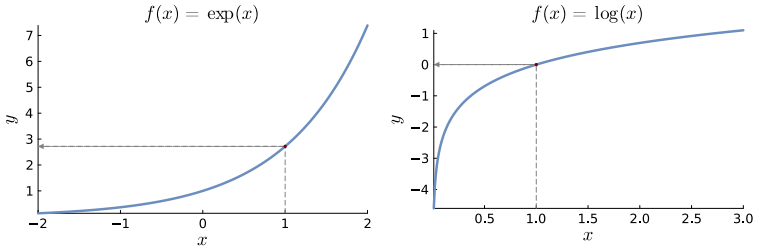

Figure 1.13: The exponential function $f(x) = \exp(x)$ (left) and the natural logarithm function $f(x) = \ln(x)$ (right).

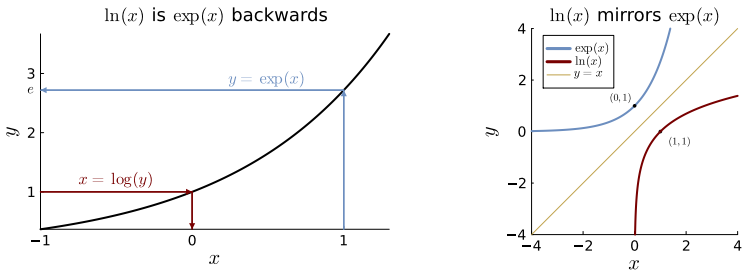

Figure 1.14: The natural logarithm function $\ln(x)$ is the inverse function of the exponential function $\exp(x)$. The left graph illustrates that an inverse function $x = f^{-1}(y)$ to $f(x)$ corresponds to going backwards from the y-axis down to the x-axis. The right graph shows that a function $y = f(x)$ and its inverse $x = f^{-1}(y)$ mirror each other in the line $y = x$.

A bijective function $f(x)$ has an **inverse function** $f^{-1}(y)$ that

inverse function

maps elements in the codomain back to elements in the domain; see Figure 1.15. Note that we used variable y as the input to the inverse function, since the output of the original function $f(x)$ is y. The actual name used as arguments to functions is not important, so we can also say that $f^{-1}(\cdot)$ is the inverse function of $f(\cdot)$, or even that f^{-1} is the inverse of f. The inverse function $f^{-1}(y)$ is defined such that the composition of f and f^{-1} is the identity function $y = x$; that is, the inverse function f^{-1} is defined as the function that satisfies $f^{-1}(f(x)) = x$ for all $x \in \mathcal{X}$. Symbolically, we have the equivalence:

$$y = f(x) \quad \Longleftrightarrow \quad x = f^{-1}(y)$$

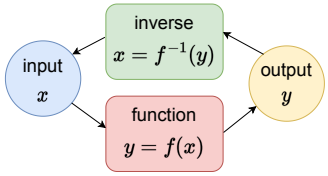

Figure 1.15: Illustration of the inverse function $x = f^{-1}(y)$.

Example: The inverse function of the exponential function $f(x) = \exp(x)$ is the natural logarithm function $f^{-1}(y) = \log(y)$; see Figure 1.13. This follows from the very definition of the natural logarithm, where $\ln(e^x) = x$ since the natural logarithm of the number e^x is the exponent x. The left graph in Figure 1.14 illustrates this inverse log-exp pair, and how the output from an inverse function to $f(x)$ are obtained by pulling elements from $y \in \mathcal{Y}$ *backward* down via $f(x)$ to $x \in \mathcal{X}$. The right graph of Figure 1.13 illustrates how the graph of f^{-1} is the mirror image of f in the line $y = x$; this mirroring property is the visualization of the defining property $f^{-1}(f(x)) = x$ of an inverse function.

EXERCISES

Functions

1. Some inverse function problem.

1.11 *Multivariable and multi-output functions*

Functions can accept more than one input. For example, the function $z = f(x, y) = x + y$ takes the two numbers x and y and return their sum as a single output z; see Figure 1.16. A function with two inputs is often called a **bivariate function**. Note that we are here using the symbol y for one of the inputs while z is now the output. The letters x, y and z are of course just dummy variables, and we could have used any other letters. The same function could therefore have been written as $y = f(x_1, x_2)$, where x_1 and x_2 are the two inputs and y is the output.

bivariate function

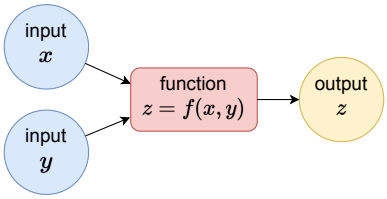

Figure 1.16: Illustration of a bivariate function $z = f(x, y)$ with two inputs x and y that together produce one output z.

Example: The Gaussian bell curve in (1.3) can be generalized to have two inputs. In the special case with two independent random

variables (see Chapter Probability) the density function is of the form

$$f(x_1, x_2) = \frac{1}{2\pi} \exp\Big(-\frac{1}{2}(x_1^2 + x_2^2)\Big). \tag{1.4}$$

The right hand graph of Figure 1.17 plot this function as a **surface plot** where function values are marked out on vertical axis (often called the z-axis in a 3D-plot) and also indicated by the darkness of the blue color on the surface. Alternatively, a two-dimensional function can be visualized in a **contour plot** where slices horizontal slices of the function are shown as two-dimensional level contours, see the right graph in Figure 1.17. The function values along a given contour have the exact same function value $f(x_1, x_2)$.

surface plot

contour plot

In the case with a function $y = f(x)$ of a single input x, we used the notation $x \in \mathcal{X}$ to denote the domain of the function. In the case with two inputs x and y we can often write the domain as $\mathcal{X} \times \mathcal{Y}$, where

$$\mathcal{X} \times \mathcal{Y} = \{(x, y) : x \in \mathcal{X} \text{ and } y \in \mathcal{Y}\}$$

is the **Cartesian product** of the two sets $\mathcal{X}$ and $\mathcal{Y}$, i.e. the set of pairs (x, y), where $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. The domain for a bivariate function does not have to be Cartesian product of two sets, it can for example be the subset of pairs (x, y) such that $x^2 + y^2 < 1$; this is the set of all points inside a circle with radius 1 in the xy-plane.

Cartesian product

More generally, a function $y = f(x_1, x_2, \ldots, x_k)$ can have k inputs that together return a single output y. An example is the sample mean

$$\bar{x} = f(x_1, x_2, \ldots, x_n) = \frac{x_1 + x_2 + \ldots + x_n}{n}$$

which can be seen as a function with n input arguments, one for each data observation, that returns the single output $\bar{x}$. A function with multiple input variables is often called a **multivariable function**.

multivariable function

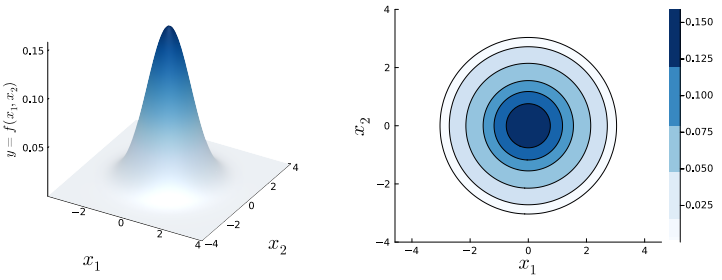

Figure 1.17: Plot of the two-dimensional Gaussian density function in (1.4) as a surface plot (left) and level contour plot (right), where the function values along a given contour have the same function value $f(x_1, x_2)$.

A function can also return more than one *output* value, for example $(y_1, y_2) = (x^2, 2x) = \mathbf{f}(x)$, meaning that the first output y_1 equals

the squared input x^2 and the second output variable y_2 is $2x$. The function was written with a bold letter **f** to indicate that it returns a *vector*, i.e. an object containing more than one number; see the Section 1.18 for more on the vector concept. All of this can of course be generalized to more than two outputs. A function with multiple output variables is often called a **vector-valued function** or **multi-output function**.

vector-valued function

multi-output function

Finally, a function can have multiple inputs $x_1, x_2, \ldots, x_k$ and multiple outputs $y_1, y_2, \ldots, y_p$, which would give a **system of equations**

system of equations

$$\begin{aligned} y_1 &= f_1(x_1, x_2, \ldots, x_k) \\ y_2 &= f_2(x_1, x_2, \ldots, x_k) \\ &\vdots \\ y_p &= f_p(x_1, x_2, \ldots, x_k) \end{aligned}$$

EXERCISES

Functions

1. Some multi-dimensional problem.

1.12 *Limits of sequences and functions*

In this section we will introduce the concept of a **limit** of a sequence or a function. The limit concept is used in the definition of the derivative and integral, and is also the basis for analyzing the properties and performance of statistical methods in large datasets.

Limit of a sequence

A **sequence** is ordered collection of numbers $x_1, x_2, \ldots, x_n$ that are indexed by the natural numbers $n = 1, 2, \ldots$. For example, the so called harmonic sequence $x_n = \frac{1}{n}$ is the collection of numbers $1, \frac{1}{2}, \frac{1}{3}, \ldots$ and so on. Another example is the sequence

sequence

$$x_n = \left(1 + \frac{1}{n}\right)^n.$$

A third example is the sequence $x_n = \log(n)$, which is the collection of numbers $\log(1) = 0, \log(2), \log(3), \ldots$. As a final example, we have the sequence $x_n = \sin(n/5)$.

It is often of interest to explore the behavior of a sequence as n gets larger and larger, i.e. as $n \to \infty$. Some sequences stabilize at a certain value as n grows large; we say that a sequence **converges**.

converges

Other sequences **diverge** to $-\infty$ or ∞, or forever oscillate between two or more values without ever settling down. Figure 1.18 plots the above four example sequences. The sequences in the top row both seem to converge as n approaches infinity, while the sequence in the bottom row diverges (bottom left), or oscillates between two values (bottom right).

diverge

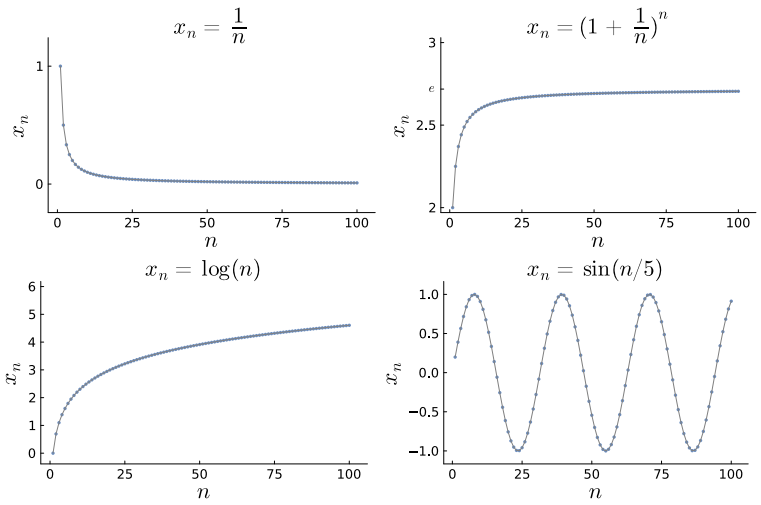

Figure 1.18: For examples of sequences with individual elements plotted as dots with a connecting line for visibility. The sequences in the top row seem to converge as n approaches infinity, while the sequence in bottom left graph seems to slowly diverge to ∞ and the sequence in the bottom right oscillates in a periodic fashion.

Here is an informal definition of a limit of a sequence:

Definition (informal)**.** *A sequence x_n approaches the **limit** L as $n \to \infty$ if x_n can be made arbitrarily close to L by choosing a large enough n. We write the limit as*

$$\lim_{n \to \infty} x_n = L$$

The following formal definition of a **limit of a sequence** makes the meaning of the vague phrase *arbitrarily close* more rigorous. The definition is a bit technical, but it is important to understand the concept of a limit since it is used in many places in statistics and machine learning; it for example the basic idea behind stochastic convergence, which we will meet in Chapter Convergence and the central theorems.

limit of a sequence

Definition. *A sequence x_n has a **limit** L if for any $\varepsilon > 0$ there exists a natural number N such that for all $n \geq N$ we have*

$$|x_n - L| < \varepsilon.$$

We write this as

$$\lim_{n\to\infty} x_n = L$$

or alternatively as

$$x_n \to L \text{ as } n \to \infty$$

Figure 1.19 illustrates the limits of the two sequences in the top row of Figure 1.18. The left graph shows that the harmonic sequence $x_n = 1/n$ converges to zero

$$\lim_{n\to\infty} \frac{1}{n} = 0$$

while the right graph shows the sequence $x_n = \left(1 + \frac{1}{n}\right)^n$ converging to Euler's number $e \approx 2.7183$,

$$\lim_{n\to\infty} \left(1 + \frac{1}{n}\right)^n = e$$

The red line in the graph is the limit of the sequence and the black lines are the ε-neighborhoods around the limit; that is, the condition $|x_n - L| < \varepsilon$ gives the ε-intervals $x_n \in (L - \varepsilon, L + \varepsilon)$. The concept of a limit implies that no matter how intolerant one is to deviations from the limit L, i.e. no matter how small ε is, there is a point N in the sequence such that all points x_n for $n \geq N$ are inside the ε-neighborhood.

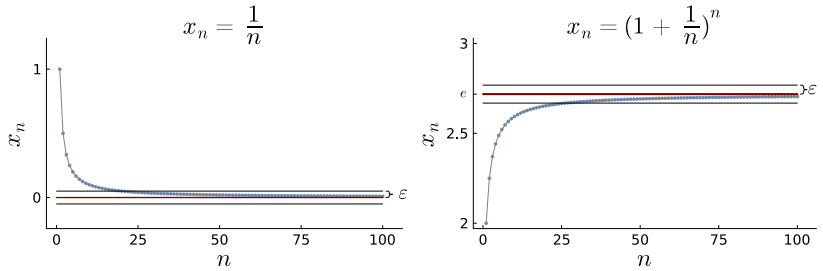

Figure 1.19: Illustration of the limit of a sequence x_n as n approaches infinity. The left graph shows the harmonic sequence $x_n = 1/n$ that converges to zero, while the right graph shows the sequence $x_n = \left(1 + \frac{1}{n}\right)^n$ that converges to e. The red line is the limit and the black lines are the ε-neighborhoods around the limit.

Example: We can use the formal definition of a limit to show that the harmonic sequence $x_n = 1/n$ converges to zero. We need to show that for any $\varepsilon > 0$ there exists a natural number N such that for all $n \geq N$ we have $|x_n - 0| < \varepsilon$. That is, we need that $|1/n - 0| < \varepsilon$, or

equivalently that $1/n < \varepsilon$, i.e. $n > 1/\varepsilon$. So, setting $N = \lceil 1/\varepsilon \rceil$ gives us the desired result, where the ceiling function $\lceil \cdot \rceil$ rounds up to the nearest integer.

EXAMPLE: Consider the sequence $x_n = a \cdot r^n$, where $-1 < r < 1$ and a is a constant and $n \in 0, 1, 2, \ldots$; note that the first element in x_0 here, i.e. the sequence starts with index 0. This sequence converges to zero as n approaches infinity. We can construct another sequence from this sequence by summing the n first elements:

$$s_n = \sum_{k=0}^{n} x_n = \sum_{k=1}^{n} a \cdot r^k = a + ar + ar^2 + \ldots \tag{1.5}$$

Sequences built up by summing elements are called **series**. The particular series in (1.5) is called the **geometric series**. Does the geometric series s_n converge, and if so, to what limit? Theorem 1.12 gives the result.

series

geometric series

Theorem 1. *If $a \neq 1$ we can write the **geometric series** as*

$$s_n = \sum_{k=0}^{n} a \cdot r^k = a \frac{1 - r^{n+1}}{1 - r}$$

an for $-1 < r < 1$, the series has the limit

$$\lim_{n \to \infty} s_n = \sum_{k=0}^{\infty} a \cdot r^k = a \frac{1}{1 - r}.$$

Finally, the next theorem box states that the Euler number $e \approx 2.71828$ is the limit of a particular series.

Theorem 2. *Euler's number e can be expressed as*

$$e = \lim_{n \to \infty} \sum_{k=0}^{n} \frac{1}{k!} = \sum_{k=0}^{\infty} \frac{1}{k!}$$

where $k! = k(k-1) \cdots 2 \cdot 1$ is the factorial of k.

Limit of a function

This far we have evaluated our functions at concrete values $f(a)$ where a is a given value. We often have to think about the value of a function $f(x)$ as x gets closer and closer to a, but perhaps never quite reach it: we write this as $x \to a$. This is very similar to a limit of a sequence x_n as $n \to \infty$, but never quite reach infinity, and the

same type of limit concept can be used for functions. Here are two examples.

EXAMPLE: Consider the function $f(x) = \frac{a^x-1}{x}$ for some constant $a > 0$. We cannot compute $f(0)$ since division by zero is not defined. What if we let x get closer and closer to zero? Let us try this for $a = 2$; we then have $f(0.01) \approx 0.69556$, $f(0.001) \approx 0.69339$, $f(0.0001) \approx 0.69317$ and $f(0.00001) \approx 0.69315$, so it seems that $f(x) = \frac{a^x-1}{x}$ settles down somewhere around 0.69315 when $a = 2$. It can be shown that for any $a > 0$, the function $f(x) = \frac{a^x-1}{x}$ settles down at exactly $\ln(a)$ as x approaches zero. This is illustrated in Figure 1.20, where the gap in the function at $x = 0$ symbolizes that the function is not defined at that point. For $a = 2$ we have $\ln(2) \approx 0.69315$, which matches our previous calculations. We write this symbolically as

$$\lim_{x \to 0} \frac{a^x - 1}{x} = \ln(a)$$

Note that the **limit point** $x = 0$ does not necessarily belong to the domain of $f(x)$.

limit point

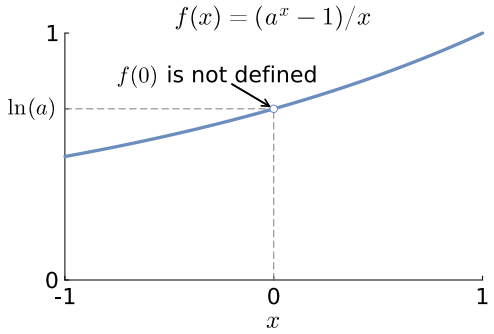

Figure 1.20: Illustration that the function $f(x) = \frac{a^x-1}{x}$ for $a > 0$ has the limit $\ln(a)$ as x approaches zero.

EXAMPLE: Consider the function $f(x) = \frac{\sin(x)}{x}$, where $\sin(x)$ is the periodic sine function plotted in left graph in Figure 1.21. What happens with $f(x)$ when x grows really large? Let us try some values: $f(1) = \sin(1)/1 \approx 0.84147$, $f(10) = \sin(10)/10 \approx -0.05440$, $f(100) = \sin(100)/100 \approx -0.00506$, $f(1000) = \sin(1000)/1000 \approx 0.00083$. It seems that the function $\frac{\sin(x)}{x}$ settles down at zero as x grows large; see the right graph in Figure 1.21. It can indeed be formally shown that

$$\lim_{x \to \infty} \frac{\sin(x)}{x} = 0.$$

We say that the function $\frac{\sin(x)}{x}$ *converges* to zero as x approaches infinity. This type of limit is called a **limit at infinity**; such limits are common in statistics, where the performance of a statistical procedure is often analyzed mathematically as the number of observations

limit at infinity

n approaches infinity. Of course, we never have infinitely many data points, but this idealized setup typically provides a good approximation of the performance in large datasets.

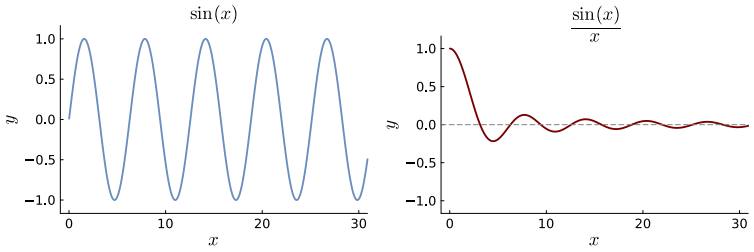

Figure 1.21: The sine function $f(x) = \sin(x)$ (left) and the damped sine wave $f(x) = \frac{\sin(x)}{x}$ (right).

The formal definition of a limit a function is quite a mouthful, so let us first give an informal definition.

Definition (informal)**.** *A function $f(x)$ approaches the **limit** L as x approaches a if $f(x)$ can be made arbitrarily close to L by an x close enough to a. This is written as*

$$\lim_{x \to a} f(x) = L$$

An alternative notation for the limit of a function is $f(x) \to L$ as $x \to a$.

The formal definition of a limit make precise what we mean by the phrase '*$f(x)$ can be made arbitrarily close to L by an x close enough to a*'. Take a deep breath. Here we go:

Definition. *A real-valued function $f(x)$ with domain $\mathcal{X}$ has a **limit** L at the point a if given any $\varepsilon > 0$ there exists some $\delta > 0$ such that for all $x \in \mathcal{X}$ satisfying*

$$0 < |x - a| < \delta$$

we have

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

We write this as

$$\lim_{x \to a} f(x) = L$$

The (ε, δ)-construction in the definition of a limit may be a little intimidating, but is quite ingenious. Think of it like this:

- no matter how intolerant a person is to approximation errors (this is the '*for any ε*' part)
- we can always move x close enough to a to make the approximation acceptable (this is the '*there exists some δ*' part).

Here is another important limit

$$\lim_{x\to\infty} \frac{x^p}{b^x} = 0, \qquad \text{for any real } p \text{ and } b > 1.$$

This shows that the exponential function b^x eventually grows faster than the power function x^p regardless of how large the exponent p is. This observable widget lets you try this out interactively. Since a polynomial function is built up from power functions, this result is often stated as '*the exponential function grows faster than any polynomial*'.

EXERCISES

Limits

1. Consider the function $f(x) = \frac{x^2-1}{x-1}$. Use a calculator or a computer to compute $f(x)$ for x-values increasing close to the point $x = 1$. Do you think the function has a limit at $x = 1$, and if so which limit?
2. Calculate $\lim_{x\to 1} \frac{x^2-1}{x-1}$.
3. Explore numerically and then show formally that

$$\lim_{x\to\infty} \frac{2x^2 - 3x + 1}{3x^2 + 4} = \frac{2}{3}$$

1.13 *Continuous functions*

We often care about how *smooth* a function is. There are many different mathematical notions of smoothness, and we will see a more detailed view in the next section. A basic notion of smoothness for a function is that a small change in x leads to a small change in the function value $f(x)$, i.e. that the function does not have any abrupt jumps. The following defintion of a **continuous function** tries to capture this idea.

continuous function

> **Definition.** *A function $f(x)$ is **continuous** at $x = a$ if*
>
> $$\lim_{x\to a} f(x) = f(a)$$

Recall the definition of a *limit*: the function $f(x)$ approaches the value $f(a)$ as x *approaches* a. If the function $f(x)$ has a jump at $x = a$, then the limit $\lim_{x\to a} f(x)$ will not be equal to $f(a)$, and the function is **discontinuous** at $x = a$. A function that is continuous for all x in its domain is called a **continuous function** or a function that is **everywhere continuous**.

discontinuous

continuous function

everywhere continuous

EXAMPLE: The function $f(x) = 2x^2 + 0.5x^3$ plotted to the left in Figure 1.22 is continuous on the domain $[-2, 3]$.

EXAMPLE: The function to the right in Figure 1.22 with domain $\mathcal{X} = [-2, 3]$ is given by

$$f(x) = \begin{cases} x^2 & \text{for } -2 \leq x < 1 \\ 2 + x^2 & \text{for } 1 \leq x < 2 \\ 6 - 2(x-2) & \text{for } 2 \leq x \leq 3 \end{cases}$$

It is continuous for all points in the two intervals $x \in [-2, 1)$ and $x \in (1, 3]$, but not in the point $x = 1$, where it jumps from the function value 1 *just before* the point $x = 1$ to the value 3 at $x = 1$. The open circle over $x = 1$ is used to symbolize that the function does not actually attain that value (its function value at $x = 1$ is 3), it is only close to that value *just before* reaching $x = 1$ from the left. The function has a sharp kink at $x = 2$, but is continuous at that point. However, in the next section on differentiation we will learn that such a kink is a form of non-smoothness.

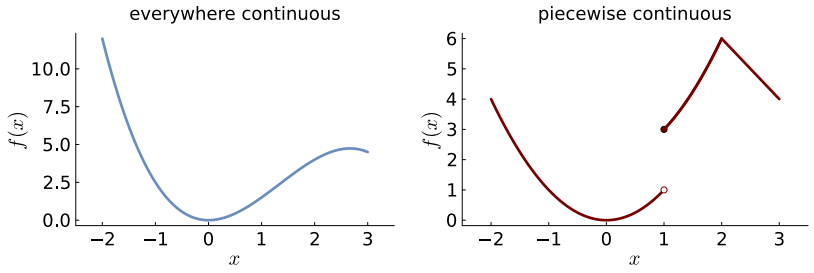

Figure 1.22: Graph of the everywhere continuous function $2x^2 + 0.5x^3$ (left) and the piecewise continuous function in (1.13) (right). The function to the right is discontiuous at $x = 1$ with a jump from the value 1 *just before* the point $x = 1$ (symbolized by the lower void point over $x = 1$) to the value $f(1) = 3$ (symbolized by the open circle over $x = 1$). The function has a sharp kink at $x = 2$, but is continuous at that point.

EXAMPLE: The function $f(x) = \frac{1}{x}$ is not continuous at $x = 0$ since $\lim_{x \to 0} \frac{1}{x}$ does not exist; the function grows to infinity as $x \to 0$.

In the chapter on Probability we will encounter *distribution functions* for random variables. One of the defining properties of a distribution function is that it is **right-continuous**, meaning that they are continuous at any point $x = a$ when approached *from the right*. This directional continuity is written as the right-sided limit

right-continuous

$$\lim_{x \to a^+} f(x) = f(a)$$

where the plus sign $(+)$ above the limit point a means that we approach a from the right, which may perhaps be visualized as: $a \leftarrow x$. Similarly, we say that a function is **left-continuous** if

left-continuous

$$\lim_{x \to a^-} f(x) = f(a)$$

where the minus sign (−) above the limit point a means that we approach *a from the left*. Figure 1.23 illustrates. A function is continuous at a if and only if it is both right-continuous and left-continuous at that point.

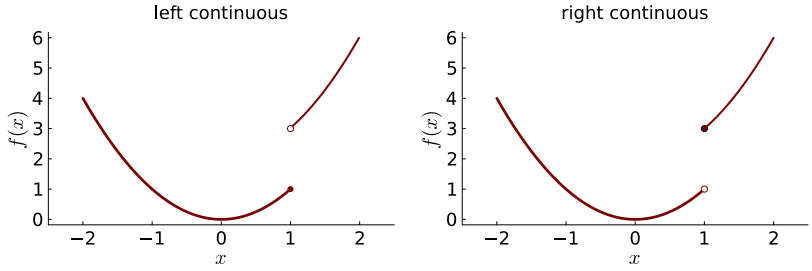

Figure 1.23: Illustration of a function that is left-continuous (left) and right-continuous (right).

EXERCISES

Continuous functions

1. Is the function

$$f(x) = \begin{cases} 0 & \text{for } x \leq 0 \\ 1 & \text{for } x > 0 \end{cases}$$

continuous, left-continuous or right-continuous at $x = 0$?

1.14 *Differentiation*

Rate of change of a function

The **rate of change** of a function $f(x)$ tells us how quickly the function changes when x changes. For a linear function $f(x) = k + bx$, this rate of change is exactly the **slope** coefficient b. To see this, let $\Delta x = x_2 - x_1$ be a change in the input x from a point x_1 to another point x_2. Let $\Delta y = y_2 - y_1$ be the corresponding change in the function output, where $y_1 = f(x_1)$ and $y_2 = f(x_2)$. Then, for a linear function, the **average rate of change** is

rate of change

slope

$$\frac{\Delta y}{\Delta x} = \frac{y_2 - y_1}{x_2 - x_1} = \frac{(k + b \cdot x_2) - (k + b \cdot x_1)}{x_2 - x_1} = \frac{b(x_2 - x_1)}{x_2 - x_1} = b$$

Importantly, for a linear function $f(x) = k + bx$, the effect of a Δx change is the **same** value b regardless of which x value we start at; this is illustrated in left graph of Figure 1.24.

The rate of change of a **nonlinear function** $f(x)$ is *not* the same for all x. A nonlinear function can change a lot for some x-values and be

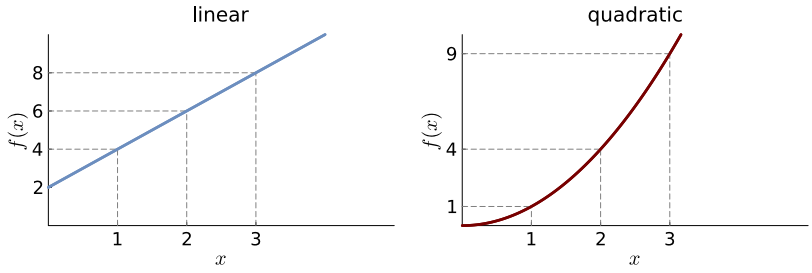

Figure 1.24: A linear function $2 + 2x$ (left) has constant rate of change for all x, for example the changes of x from 0 to 1 to 2 all increase the function with 2 units. In contrast, the rate of change for a nonlinear function (right) depends on which x the change is initiated from; a change from $x = 1$ to $x = 2$ increases the function output with 3 units while changing from $x = 2$ to $x = 3$ increases the function output with 5 units.

nearly constant at other x-values. For example, consider the square function $f(x) = x^2$ which is plotted in the right graph of Figure 1.24, where

- a change from $x = 1$ to $x = 2$ changes the function value from $f(1) = 1$ to $f(2) = 4$.
- a change from $x = 2$ to $x = 3$ changes the function value from $f(2) = 4$ to $f(3) = 9$.

How much the square function changes when we change its input by $\Delta x = 1$ clearly depends on where we are on the x-axis.

Before explaining how we measure the *local* rate of change of a nonlinear function, it is useful to express the average rate of change $\frac{\Delta y}{\Delta x}$ so that we see the function $f(x)$ explicitly in the expression. Let the function input start at some value x and then move Δx units to another value $x + \Delta x$. The change along the y-axis is then

$$\Delta y = f(x + \Delta x) - f(x)$$

We can therefore write the average rate of change in terms of the function as

$$\frac{\Delta y}{\Delta x} = \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

It is common to use the letter h instead of Δx to denote a change along the x-axis, so the **average rate of change** between $x = a$ and $x = a + h$ is written

average rate of change

$$\frac{f(a + h) - f(a)}{h}$$

Figure 1.25 plots the exponential function $f(x) = \exp(x)$ (blue curve) with the two evaluation points at a and $a + h$ plotted as red dots. The red line that connects the two evaluation points is called a **secant line**. The slope of the secant line is the average rate of change of the function $f(x)$ between a and $a + h$.

secant line

The derivative

The **derivative** of a function $f(x)$ at $x = a$ is defined as the average

derivative

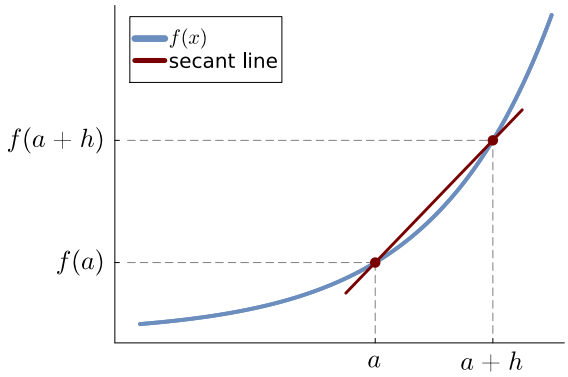

Figure 1.25: Secant

rate of change

$$\frac{f(a+h)-f(a)}{h}$$

where the change h in x is extremely small. In fact, the definition of a derivative lets h approach zero, using the concept of a *limit* from Section Limits of sequences and functions. Here is the formal definition.

Definition. *The **derivative** of a function $f(x)$ at $x = a$ is*

$$f'(a) = \lim_{h \to 0} \frac{f(a+h)-f(a)}{h}$$

provided that the limit exists.
*If the limit exists we say that $f(x)$ is **differentiable** at $x = a$.*

The derivative is therefore the slope of the secant line in Figure 1.25 as $h \to 0$. Figure 1.26 illustrates how the secant line settles down, or converges, to a **tangent line** as $h \to 0$. The slope of the tangent line is the derivative $f'(a)$ at $x = a$ and measures the **instantaneous rate of change** of the function $f(x)$ at the given $x = a$. The tangent line is the best linear approximation of the function around $x = a$. Figure 1.27 plots the secant and tangent lines. This observable widget illustrates the derivative with an interactive plot for several common functions. The little blip ′ in the notation $f'(a)$ is called a *prime*. So the symbol f' is often read as 'f prime'.

tangent line

instantaneous rate of change

If we trace out the derivative $f'(a)$ over all points a values in the domain where the derivative exists, the derivative is itself a function of x; the symbol $f'(x)$ denotes that function, and is a function that can be evaluated for any x-value to obtain the derivative at that point. See for example the top left graph of Figure 1.28 which plots the square function $f(x) = x^2$ and its derivative. See also this observable widget.

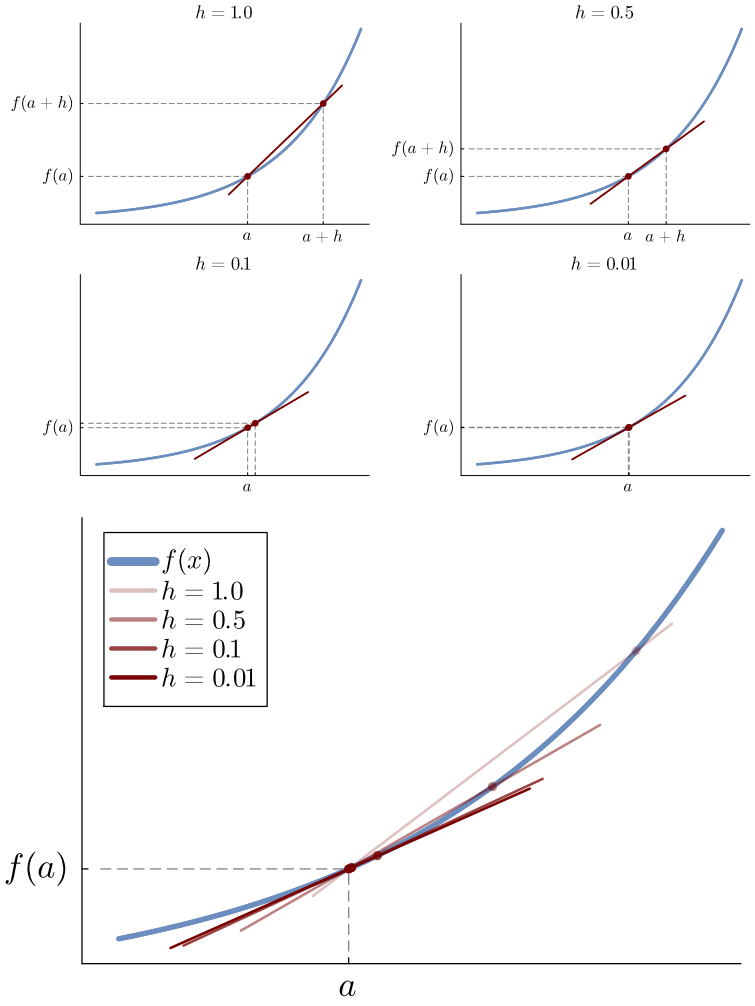

Figure 1.26: Illustration the derivative as the limiting average rate of change as $h \to 0$. The blue curve is the function and the red line is the secant line between a and $a + h$. The slope of the secant line approaches the derivative, i.e. the slope tangent line, as h approaches zero. The graph at the bottom shows all secant lines in the same graph.

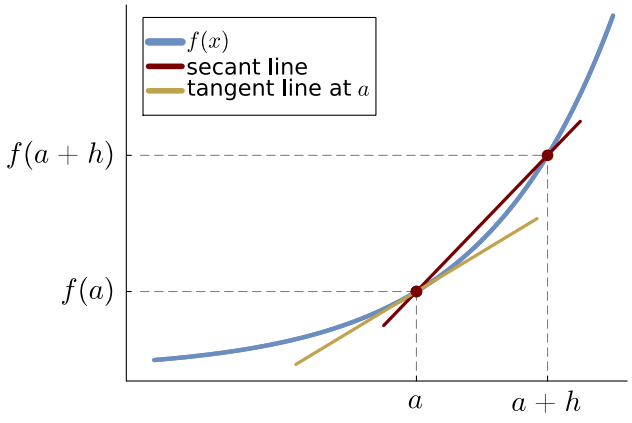

Figure 1.27: Illustration of the secant line (red) and tangent line (yellow) at point $x = a$ for the exponential function.

EXAMPLE: Let us try to use the definition to compute the derivative $f'(x)$ of the square function $f(x) = x^2$, and evaluate the derivative at $x = 2$. From the definition above

$$f'(x) = \frac{f(x+h) - x}{h} = \frac{(x+h)^2 - x^2}{h} = \frac{(x^2 + 2xh + h^2) - x^2}{h} = 2x + h$$

which clearly approaches $2x$ when $h \to 0$. So the derivative of the square function $f(x) = x^2$ is $f'(x) = 2x$. The derivative at $x = 2$ is therefore $f'(2) = 2 \cdot 2 = 4$.

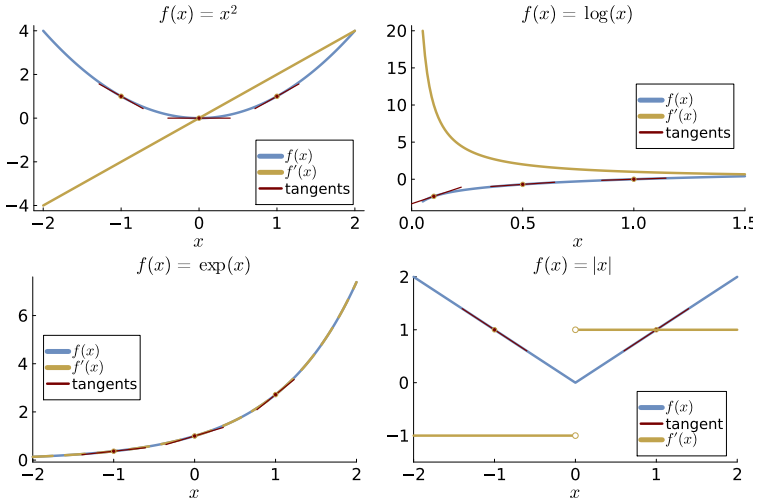

Figure 1.28: Four common functions (blue curve) with their derivative functions (yellow curve) and tangents (red lines) at some selected x. The derivative functions are: $f'(x) = 2x$ (for the square function), $f'(x) = 1/x$ (for the log function), $f'(x) = \exp(x)$ (for the log function) and $f'(x) = \text{sign}(x)$ (for the absolut value function). Note that for the exponential function we have $f'(x) = f(x)$, so the function and its derivative are completely overlapping. The derivative at $x = 0$ does not exist for the absolute value function which is represented by the void circles.

Note that the limit in the definition of the derivative may not exist at some x values, for example at points where the function jumps or has sharp corners. The derivative function $f(x)$ is then undefined for those non-differentiable x-values. One example is the absolute value function $f(x) = |x|$, depicted in the lower right graph of Figure 1.28 which has derivative

$$f'(x) = \begin{cases} -1 & \text{if } x < 0 \\ 1 & \text{if } x > 0 \\ \text{undefined} & \text{if } x = 0. \end{cases}$$

Note that the absolute value function is not diffentiable at $x = 0$, where the function has a sharp corner and its derivative immediately switches from -1 for negative x to 1 for positive x; see Figure 1.28. Recall the concept of continuity of a function from Section Referencessec:continuity. The absolute value function is continuous for all x, and in particular at $x = 0$. So a function with a kink at can be continuous, but not differentiable at that point. Differentiability is a stronger smoothness requirement than continuity.

The derivative and its tangent line at some $x = a$ can be used in a

linear approximation of the function $f(x)$ around $x = a$

$$f(x) \approx f(a) + f'(a)(x - a).$$

The approximation becomes more accurate the closer x is to a; it is a *local* linear approximation around $x = a$. This idea can be generalized to include so called higher order derivative in the Taylor approximation discussed in Section Function approximation below.

Rules of differentiation

The formal definition of the derivative as a limit is rarely used in practical work. There are instead **rules of differentiation** that can be used quite easily (of course, these rules were once proved using the formal definition of a derivative as a limit). For example, the derivative of the square function, as derived above, is a special case of the **power function derivative rule** that says that

power function derivative rule

The function $f(x) = x^p$ for $p \in \mathbb{R}$ has derivative $f'(x) = px^{p-1}$.

Using the power rule we immediately see, for example, that the cubic function $f(x) = x^3$ has derivative $f'(x) = 3x^2$. The derivatives of some elementary functions are listed in Figure 1.14. Note in particular that the derivative of the exponential function e^x is the exponential function itself, i.e. $f'(x) = e^x$. Since $\frac{1}{x} = x^{-1}$, the reciprocal rule $\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{x} = -\frac{1}{x^2}$ in Figure 1.14 is a special case of the power rule with $p = -1$.

Many functions are combinations, e.g. sums, products or function compositions, of elementary functions. For example, the 2nd degree polynomial $f(x) = b_0 + b_1 x + b_2 x^2$ is a sum of the constant function $f(x) = b_0$, the linear function $g(x) = b_1 x$ and the quadratic function $h(x) = b_2 x^2$. There are very useful differentation rules for combinations of functions; to express these rules, it is convenient to use an alternative notation for the derivative of a function than the $f'(x)$ used so far. The alternative notation tries to mimic the notation used above for the average rate of change, $\frac{\Delta y}{\Delta x}$, but with the Δ symbol (which is capital D in the greek alphabet) replaced by the smaller d symbol; the idea is that derivatives are rates of change for a tiny Δx change. The following three types of notations all denote the same derivative function

$$f'(x) \qquad \frac{\mathrm{d}f(x)}{\mathrm{d}x} \qquad \frac{\mathrm{d}}{\mathrm{d}x}f(x)$$

With this alternative notation for the derivative in place, we can write down the **sum rule for derivatives** as

sum rule for derivatives

$$\frac{\mathrm{d}}{\mathrm{d}x}\big(f(x) + g(x)\big) = f'(x) + g'(x).$$

Derivatives of elementary functions

$\frac{\mathrm{d}}{\mathrm{d}x}a = 0$ for constant a
$\frac{\mathrm{d}}{\mathrm{d}x}(a+bx) = b$
$\frac{\mathrm{d}}{\mathrm{d}x}x^p = px^{p-1}$
$\frac{\mathrm{d}}{\mathrm{d}x}e^x = e^x$
$\frac{\mathrm{d}}{\mathrm{d}x}\ln(x) = \frac{1}{x}$
$\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{x} = -\frac{1}{x^2}$
$\frac{\mathrm{d}}{\mathrm{d}x}a^x = a^x\ln(a)$
$\frac{\mathrm{d}}{\mathrm{d}x}\cos(x) = -\sin(x)$
$\frac{\mathrm{d}}{\mathrm{d}x}\sin(x) = \cos(x)$

Hence, the derivative of a sum of functions is the sum of the derivatives of the functions. In the old notation this rule is a little less readable

$$(f(x)+g(x))' = f'(x)+g'(x).$$

Combining the sum rule with the rules for derivatives of elementary functions in Figure 1.14 we can for example compute the derivative of the function $f(x) = x^2 + e^x$ as

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(x^2+e^x\right) = \frac{\mathrm{d}}{\mathrm{d}x}x^2 + \frac{\mathrm{d}}{\mathrm{d}x}e^x = 2x + e^x.$$

What if we need the derivative of a *product of functions*, $f(x)g(x)$, for two differentiable functions $f(x)$ and $g(x)$? For example, the function $x^2 \cdot e^x$ is the product of the quadratic function $f(x) = x^2$ and the exponential function $g(x) = e^x$. The **product rule for derivatives** says that

product rule for derivatives

$$\frac{\mathrm{d}}{\mathrm{d}x}\big(f(x)g(x)\big) = f'(x)g(x) + f(x)g'(x).$$

where we have used both types of notations for the derivative to get the most pleasant looking formula. We can use this rule to calculate

$$\frac{\mathrm{d}}{\mathrm{d}x}\big(x^2 \cdot e^x\big) = 2x \cdot e^x + x^2 \cdot e^x = x(2+x)e^x,$$

since the derivative of the square function is $f'(x) = 2x$ and the derivative of the exponential function is the exponential function itself, i.e. $g'(x) = e^x$.

Figure 1.14 collects the sum and product together with some other useful differentiation rules for combinations of functions. Note that both $f(x)$ and $g(x)$ must be differentiable for the rules to hold. These rules can be generalized to more than two functions, for example the derivative of a sum of three functions is the sum of the derivatives of the three functions

$$\frac{\mathrm{d}}{\mathrm{d}x}\big(f(x) + g(x) + h(x)\big) = f'(x) + g'(x) + h'(x),$$

provided all three functions are differentiable.

Derivative of a combination of differentiable functions

Constant rule	$\frac{\mathrm{d}}{\mathrm{d}x}a = 0$ for constant a
Scaling rule	$\frac{\mathrm{d}}{\mathrm{d}x}\big(a \cdot f(x)\big) = a \cdot f'(x)$ for constant a
Sum rule	$\frac{\mathrm{d}}{\mathrm{d}x}\big(f(x) + g(x)\big) = f'(x) + g'(x)$
Product rule	$\frac{\mathrm{d}}{\mathrm{d}x}\big(f(x)g(x)\big) = f'(x)g(x) + f(x)g'(x)$
Quotient rule	$\frac{\mathrm{d}}{\mathrm{d}x}\frac{f(x)}{g(x)} = \frac{f'(x)g(x) - f(x)g'(x)}{(g(x))^2}$
Reciprocal rule	$\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{g(x)} = -\frac{g'(x)}{(g(x))^2}$
Chain rule	$\frac{\mathrm{d}}{\mathrm{d}x}g(h(x)) = g'(h(x)) \cdot h'(x)$

A particularly important rule in Figure 1.14 is the **chain rule for derivatives** which is used to differentiate a *composition of functions*, $g(h(x))$. The chain rule says that (note the colors, which are explained below)

chain rule for derivatives

$$\frac{\mathrm{d}}{\mathrm{d}x}g(h(x)) = g'(h(x)) \cdot h'(x)$$

In the terminology for composite functions from Section 1.9, the chain rule says that

> the derivative of a composite function $g(h(x))$ is the **derivative of the outer function** $g'(x)$ evaluated at the inner function $h(x)$ multiplied with the **derivative of the inner function** $h'(x)$.

EXAMPLE: The chain rule is more useful than one might think at first. For example, the function $f(x) = e^{ax}$ can be seen as a composition of the exponential function $g(x) = e^x$ and the linear function $h(x) = ax$. Combining the chain rule with derivatives of these two component functions ($g'(x) = e^x$ and $h'(x) = a$) therefore gives

$$\frac{\mathrm{d}}{\mathrm{d}x} e^{ax} = e^{ax} \cdot a = ae^{ax}.$$

EXAMPLE: The derivative of $\log h(x)$ for some differentiable function $h(x)$ can be computed with the chain rule; here the outer function is $g(x) = \log x$ with derivative $g'(x) = \frac{1}{x}$, while the inner function is $h(x)$. The derivative is

$$\frac{\mathrm{d}}{\mathrm{d}x} \log h(x) = \frac{1}{h(x)} h'(x) = \frac{h'(x)}{h(x)}.$$

Second and higher order derivatives

As we have discussed, the derivative $f'(x)$ is itself a function of x. We can therefore calculate *the derivative of the derivative* itself. We call this the **second derivative** of $f(x)$, and denote it

second derivative

$$f''(x) = \frac{\mathrm{d}}{\mathrm{d}x} f'(x)$$

The first derivative $f'(x)$ measures how fast the function $f(x)$ changes and a positive sign of $f'(a)$ at $x = a$ means that the slope of the tangent line is positive so that the function is increasing. Similarly, the second derivative $f''(x)$ measures *how fast the first derivative* $f'(x)$ *changes*. The second derivative at $x = a$ is therefore a measure of the **acceleration** of the function $f(x)$ at the point $x = a$.

acceleration

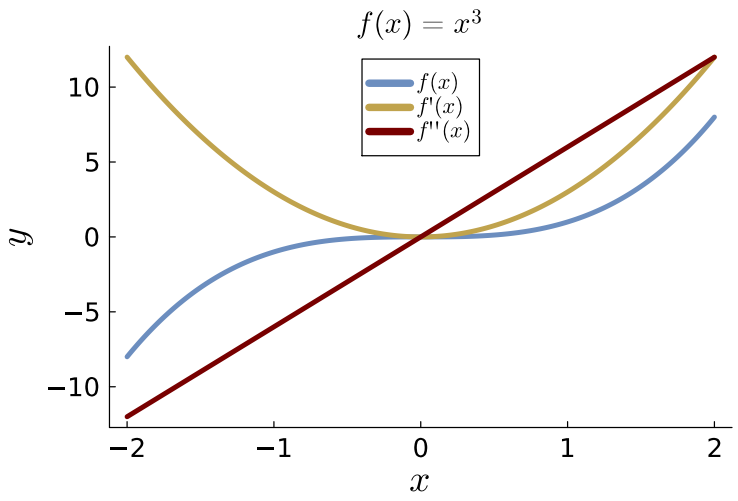

Figure 1.29: The cubic function $f(x) = x^3$ (blue) and its first derivative $f'(x) = 3x^2$ (yellow) and second derivative $f''(x) = 6x$ (red).

EXAMPLE: Consider the cubic function $f(x) = x^3$, plotted as the blue line in Figure 1.29. The first derivative of the cubic function $f(x) = x^3$ is $f'(x) = 3x^2$ and is plotted as the yellow line in Figure 1.29. The second derivative of $f(x)$ is the derivative of the first derivative, hence $f''(x) = \frac{\mathrm{d}}{\mathrm{d}x} f'(x) = \frac{\mathrm{d}}{\mathrm{d}x}(3x^2) = 6x$; this is the red line in Figure 1.29. Let us investigate three points:

- At $x = 0$ the cubic function is $f(0) = 0$ and its first derivative is $f'(0) = 0$, meaning that the tangent line is horizontal at $x = 0$; a small change in x around $x = 0$ will have no effect on the function value.
- At $x = 1$ the cubic function is $f(1) = 1$ and its first derivative is $f'(1) = 3$, meaning that the tangent line has a slope of 3 at $x = 1$; the function is increasing at $x = 1$. The second derivative at $x = 1$ is $f''(1) = 6$, meaning that the slope of the tangent line is increasing at $x = 1$. The function is therefore accelerating upwards at $x = 1$.
- At $x = -1$ the function is $f(-1) = -1$ and its first derivative is $f'(-1) = 3$, meaning that the tangent line has a slope of 3 at $x = -1$; even though the function is negative here, it is increasing since the first derivative is positive also at $x = -1$. However, the second derivative at $x = -1$ is $f''(-1) = -6$, meaning that the slope of the tangent line is decreasing at $x = -1$; the function is deaccelerating at $x = -1$.

Since the second derivative $f''(x)$ is itself a function of x, we can take the derivative of the second derivative, which we call the third derivative of $f(x)$, and denote it as $f'''(x)$ or $f^{(3)}(x)$; we can clearly continue like this to obtain **higher order derivatives**. The first and second derivatives are the most important ones, and we will concentrate on them in most of this book and in the Bayesian learning book. Third and higher order derivatives only make a brief entrance in the Taylor approximation of a function $f(x)$ in Section 1.17.

higher order derivatives

Partial derivatives of multivariable functions

Recall that a function can have more than one input variable, for example the bivariate function $z = f(x, y)$. In this section we explore a measure of how much the function changes when we change x a little, *while keeping the other input variable y constant*. Similarly, we can ask how much the function changes when we change y a little, while keeping the other input variable x constant. The **partial derivative** is the natural generalization of the derivative concept to functions with more than one input variable.

partial derivative

Definition. *The **partial derivatives** of a function $f(x, y)$ with respect to x and y are defined as*

$$f_x(x,y) = \frac{\partial}{\partial x} f(x,y) = \lim_{h \to 0} \frac{f(x+h,y) - f(x,y)}{h}$$
$$f_y(x,y) = \frac{\partial}{\partial y} f(x,y) = \lim_{h \to 0} \frac{f(x,y+h) - f(x,y)}{h}$$

provided that the limits exists.

Note that it is customary to use the symbol ∂ instead of the symbol d for partial derivatives. We do not use the prime $'$ symbol for partial derivatives, and instead indicate the differentiation variable by the subscript, so that $f_x(x, y)$ is the partial derivative with respect to x when holding y constant, and $f_y(x, y)$ is the partial derivative with respect to y when holding x constant.

Example: Consider the function $f(x, y) = -x^2y^2$. The partial derivative with respect to x is

$$f_x(x,y) = \frac{\partial}{\partial x}(-x^2y^2) = -2xy^2$$

and the partial derivative with respect to y is

$$f_y(x,y) = \frac{\partial}{\partial y}(-x^2y^2) = -2x^2y.$$

The partial derivatives at the point $(x_0, y_0) = (-1, 1)$ are $f_x(-1, 1) = 2$ and $f_y(-1, 1) = -2$. The red line in Figure 1.30 is the tangent line for the partial derivative with respect to x; the slope is indeed positive in the x-direction. The blue line is the tangent of the partial derivative with respect to y; here the slope is negative in the y-direction; note the direction of the y-axis in the plot: as y increases, the values on along the blue line decreases.

Figure 1.30 plots the two tangent lines in the x and y directions with slopes $f_x(x_0, y_0)$ and $f_y(x_0, y_0)$, respectively. We can also define a **tangent plane** to a bivariate function $f(x, y)$ at the point $(x, y) = (x_0, y_0)$. A plane is a two-dimensional generalization of a line. The tangent plane at $(x, y) = (x_0, y_0)$ is given by

tangent plane

$$f(x,y) \approx f(x_0,y_0) + f_x(x_0,y_0)(x - x_0) + f_y(x_0,y_0)(y - y_0).$$

The tangent plane is a generalization of the tangent line for univariate functions to two dimensions, and is the best linear approximation of the function $f(x, y)$ around the point (x_0, y_0). Figure 1.31 plot the tangent plane for the function $f(x, y) = -x^2y^2$ in the point $(x_0, y_0) = (-1, 1)$.

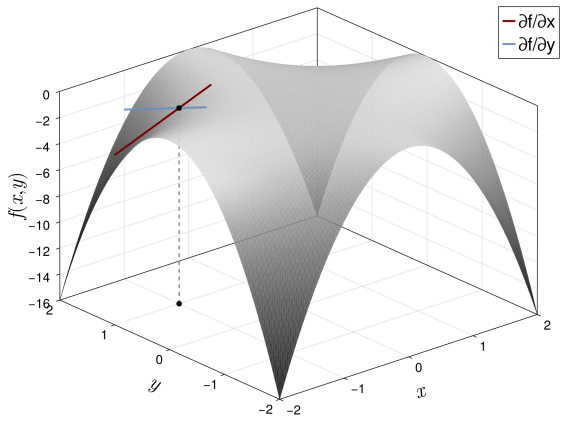

Figure 1.30: Illustration of the partial derivatives of the bivariate function $f(x, y) = -x^2y^2$ at the point $(x_0, y_0) = (-1, 1)$. The partial derivative with respect to x is the slope of the tangent line in the x-direction (red line) given $y = y_0$, while the partial derivative with respect to y is the slope of the tangent line in the y-direction (blue line) given $x = x_0$.

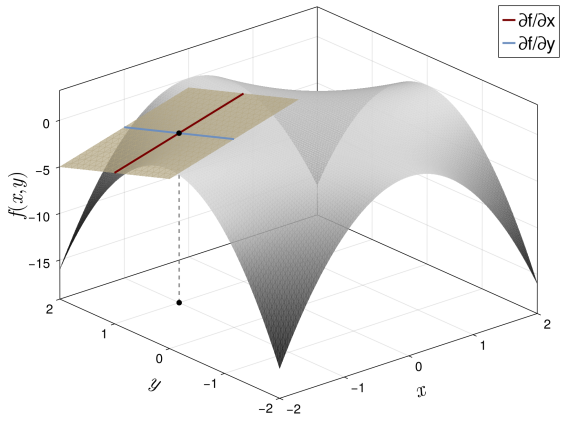

Figure 1.31: Illustration of the tangent plane of the bivariate function $f(x, y) = -x^2y^2$ at the point $(x_0, y_0) = (-1, 1)$.

For functions in one variable $f(x)$ we defined the second derivative $\frac{\mathrm{d}^2}{\mathrm{d}x^2}f(x)$ as the derivative of the derivative, $\frac{\mathrm{d}}{\mathrm{d}x}f'(x)$. We can also define **second order partial derivatives** in a similar fashion

second order partial derivatives

$$f_{xx}(x,y) = \frac{\partial^2}{\partial x^2}f(x,y) = \frac{\partial}{\partial x}f_x(x,y)$$

which is the partial derivative of the partial derivative $f_x(x,y)$. It measures the same thing as the second derivative of a single-variable function $f(x)$ but the interpretation in the multivariable case is again under the condition that the other variable y is held constant.

Finally, we define the **cross partial derivative**

cross partial derivative

$$f_{xy}(x,y) = \frac{\partial^2}{\partial y \partial x}f(x,y) = \frac{\partial}{\partial y}f_x(x,y)$$

which is obtained by first taking the partial derivative of the function $f(x,y)$ with respect to x and then with respect to y.

EXAMPLE: Let $f(x,y) = -x^2y^2$. The second partial derivative with respect to x is

$$f_{xx}(x,y) = \frac{\partial^2}{\partial x^2}f(x,y) = \frac{\partial}{\partial x}f_x(x,y) = \frac{\partial}{\partial x}(-2xy^2) = -2y^2$$

and the cross partial derivative

$$f_{xy}(x,y) = \frac{\partial^2}{\partial y \partial x}f(x,y) = \frac{\partial}{\partial y}f_x(x,y) = \frac{\partial}{\partial y}(-2xy^2) = -4xy.$$

If the second partial derivatives are continuous then

$$\frac{\partial^2}{\partial y \partial x}f(x,y) = \frac{\partial^2}{\partial x \partial y}f(x,y),$$

so it does not matter if we take the partial derivative with respect to x or y first.

EXERCISES

Differentiation

1. Find the derivative of $f(x) = 3x^2$
2. Find the derivative of $f(x) = 1 + 3x^2$
3. Find the derivative of $f(x) = 3x^2 + 2x$
4. Find the derivative of $f(x) = e^{2x}$
5. Find the derivative of $f(x) = e^{-3x}$
6. Find the derivative of $f(y) = \left(\frac{1}{1+y}\right)^2$

7. Find the derivative of $f(x) = x^2 e^x$
8. Find the derivative of $f(x) = \frac{x^2}{e^x}$
9. Find the derivative of $f(x) = x^{-2} e^x$
10. Find the first and second derivatives of $f(x) = x^3 + 2x^2 + 4$
11. Find the first and second derivatives of $f(x) = \exp(x)$
12. Find the first and second derivatives of $f(x) = \ln(x)$
13. Let $f(x) = x^2$. Explain in words the meaning of $f'(x) = 2x$ and $f''(x) = 2$ for all x
14. Let $f(x, y) = x^3 y$. Find the partial derivatives $f_x(x, y)$ and $f_y(x, y)$.
15. Let $f(x, y) = \exp(xy)$. Find the partial derivatives $f_x(x, y)$ and $f_y(x, y)$.
16. Let $f(x, y) = x^2 \log(y) e^y$. Find the partial derivatives $f_x(x, y)$ and $f_y(x, y)$.
17. Let $f(x, y) = x + xy^2$. Find the second partial derivatives $f_{xx}(x, y)$ and $f_{yy}(x, y)$ and the cross partial derivative $f_{xy}(x, y)$.

1.15 *Function optimization*

Many of the most important problems in statistics and machine learning involve finding the maximum or minimum of a function. For example, the mode of a density function is the value of the random variable that maximizes the density function; see Chapter 2. The maximum likelihood estimate (see Chapter 8) of a parameter is the value of the parameter that maximizes the likelihood function. Model like deep neural networks in machine learning are trained by minimizing a loss function, a measure how well the model fits the data. Optimization problem are common in all areas, for example a firm trying to find the how large a stock to keep for its product in order to maximize profits, or a political party deciding on how to allocate its campaign budget on different media channels. Minimization and maximimization problems are collectively known as **optimization** problems.

optimization

In this section we will show a mathematical technique for finding the minimum or maximum of a differentiable function $f(x)$. The first and second derivatives are shown to play a big role. We will also give an introduction to **numerical optimization**, where numerical computer algorithms are used to find the minimum or maximum of a function in more complicated problems.

Finding the optimum of a function with a single input

Assume that we want to find the maximum of a function $f(x)$ over a domain $x \in [a, b]$; that is we are searching for the input $x \in [a, b]$ with the largest function output $y = f(x)$. This input value is called the **maximizer** of $f(x)$ and is denoted by $x_{\max}$. It is also common to use the phrase **argument of the maximum** for $x_{\max}$, and we often write

maximizer

argument of the maximum

$$x_{\max} = \arg\max_{x \in [a,b]} f(x)$$

which is read as '$x_{\max}$ is the argument that maximizes the function $f(x)$ over the domain $[a, b]$'.

The maximizer can cleverly be found using the derivative $f'(x)$, provided that the function is smooth enough to be differentiable. Recall that the derivative measures the local slope of the function at each x, see Figure 1.32 that plots the quadratic function $f(x) = 1 - (x-1)^2$ as a blue line and the tangent lines (red lines) at the points $x = 0$, $x = 1$ and $x = 2$ (red dots). The derivative function $f'(x) = -2(x-1)$ is also plotted as a yellow line. It is clear that we can find the maximum by searching for an x where the derivative is zero, i.e. we have the condition for a maximum

$$f'(x_{\max}) = 0$$

We can therefore find the maximizer $x_{\max}$ by solving the equation $f'(x) = -2(x-1) = 0$, which has solution $x = 1$. This is called the **first-derivative test** for finding the maximum of a function. The point where the derivative is zero is often called a **critical point** of the function.

first-derivative test

critical point

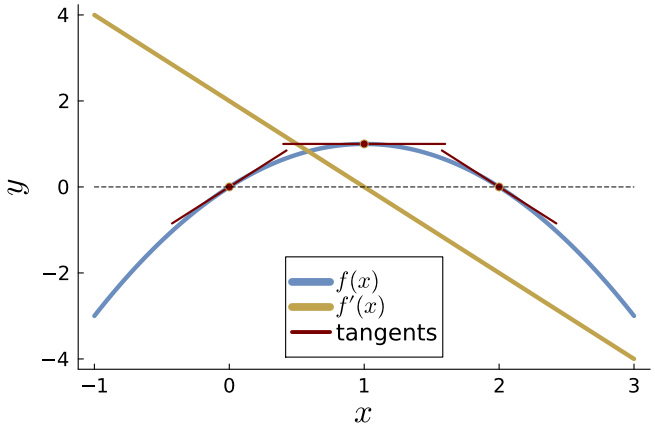

Figure 1.32: Illustration of the first derivative test for the quadratic function $f(x) = 1 - (x-1)^2$ (blue curve) with derivative $f'(x) = -2(x-1)$ (yellow line). The function has a maximum at $x = 1$ where the red tangent line has zero slope.

Not all critical points are maximizers, however. The derivative is zero also at two other types of points: at **minimizers** as in the top right graph of Figure 1.33, and inflection points as in the middle

minimizers

left graph of Figure 1.33. An **inflection point** is a point where the derivative changes sign, but which is not a minimum or maximum.

inflection point

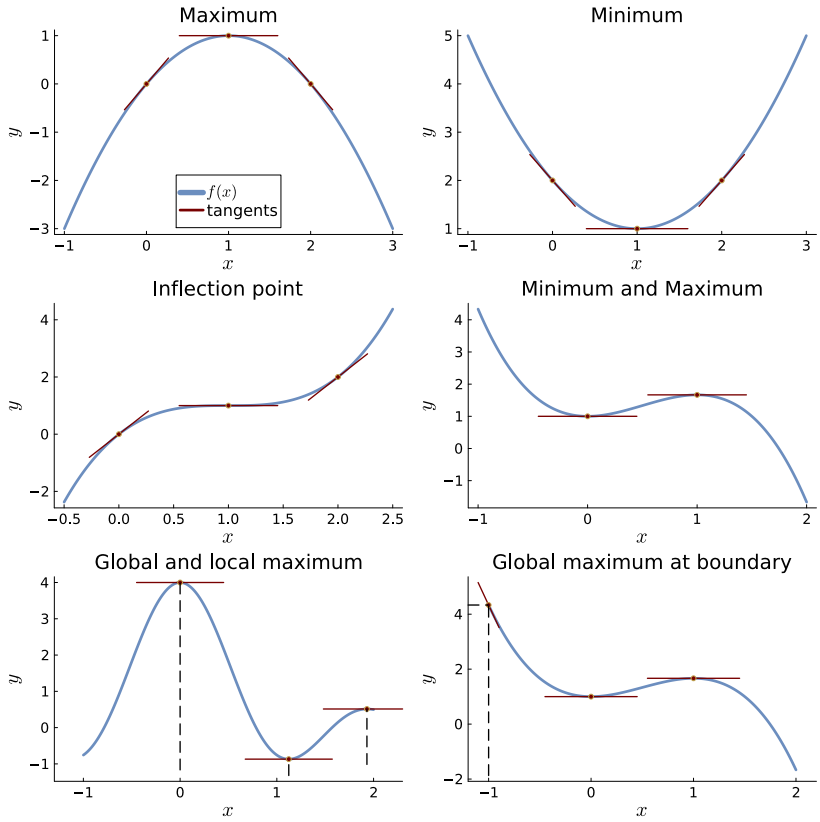

Figure 1.33: Illustrating that the first-derivative test detects a maximum of the function $f(x) = 1 - (x-1)^2$ (top left) and a minimum of the function $f(x) = 1 + (x-1)^2$ (top right). The middle left graph shows that the function $f(x) = x^3 - 3x^2 + 3x$ has an inflection point at $x = 1$. A function can also have several local minima and maxima, like the function $f(x) = 1 + 2x^2 - (4/3)x^3$ in lower left graph. Finally, the function in the lower right graph has its global maximum at the boundary of the domain $(-1, 2)$ where the derivative is not zero.

The *second-derivative test* is a way to determine whether a critical point is a maximum, minimum or an inflection point. As we saw in Section 1.14, the second derivative $f''(x)$ measures the rate of change in the derivative«s at x. If the second derivative is negative at a critical point, then that means that the first derivative is decreasing and the function is curving downwards, and the critical point is a maximum. If the second derivative is positive at a critical point, then the function is curving upwards and the critical point is a minimum. If the second derivative is zero, then the test is inconclusive and we cannot use the derivative to determine what kind of critical point we have. In summary:

Result. ***(Second-derivative test)***

If x_c is a critical point, i.e. $f'(x_c) = 0$, then

- *If $f''(x_c) < 0$ the function has a **local maximum** at $x = x_c$*
- *If $f''(x_c) > 0$ the function has a **local minumum** at $x = x_c$*
- *If $f''(x_c) = 0$ the test is inconclusive*

Let us perform the derivative test on three of the functions used in Figure 1.33:

- The function $f(x) = 1 - (x-1)^2$ with first derivative $f'(x) = -2(x-1)$ has a critical point at $x_c = 1$. Here $f''(x) = -2$ which is negative at for all x, including $x_c = 1$. Hence the critical point is a local maximizer.
- The function $f(x) = 1 + (x-1)^2$ with first derivative $f'(x) = 2(x-1)$ has a critical point at $x_c = 1$. Here $f''(x) = 2$ which is positive at $x_c = 1$, and this critical point is a local minimizer.
- The function $f(x) = x^3 - 3x^2 + 3x$ with first derivative $f'(x) = 3x^2 - 6x + 3 = 3(x-1)^2$ has a critical point at $x_c = 1$, and second derivative $f''(x) = 6x - 6$ which is $f''(1) = 0$, so the second-derivative test is inconclusive at $x_c = 1$. We know from Figure 1.33 that this an inflection point

The first derivative test detects both a **local optimum**, i.e. the optimum in some subregion, and a **global optimum**, which is the maximizer over all of the domain for the optimization. The lower left graph in Figure 1.33 shows a function with one local maximum, one local minimum and one global maximum.

local optimum

global optimum

Finally, the maximum or minimum of a function can also occur at the boundary of the domain, where the first derivative is typically non-zero so it will not be detected with the first derivative test. The lower right graph in Figure 1.33 shows a function with a global maximum at the boundary of the domain $(-1, 2)$.

The only way to make sure that the global maximum or minimum of a function has been found is to evaluate the function at all of the critical points and at the boundaries of the domain. The largest value is the global maximum and the smallest value is the global minimum.

*Finding the optimum of a multivariable function**

A similar approach can be used to find the maximum of a function with more than one input variable, for example, the bivariate func-

tion $z = f(x, y)$. The critical points of the function are the points where the partial derivatives $f_x(x, y)$ and $f_y(x, y)$ are both zero. The **first partial derivative test** is then to solve the system of two equations formed by setting the partial derivatives to zero:

first partial derivative test

$$f_x(x, y) = 0$$
$$f_y(x, y) = 0$$

for the critical points $(x = x_c, y = y_c)$. Since the **gradient** is the vector with partial derivatives, we can express the first partial derivative test as solving for the x and y that makes the gradient vector equal to the zero vector:

$$\begin{pmatrix} f_x(x, y) \\ f_y(x, y) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

The second-derivative test for a bivariate function $f(x, y)$ is based on the determinant of the Hessian matrix

$$\mathbf{H}(x, y) = \begin{pmatrix} f_{xx}(x, y) & f_{xy}(x, y) \\ f_{xy}(x, y) & f_{yy}(x, y) \end{pmatrix}$$

evaluated at the critical point (x_c, y_c). The second partial derivative test is then:

Result. ***(Second partial derivative test)***

If (x_c, y_c) is a critical point, i.e. $f_x(x_c, y_c) = 0$ and $f_y(x_c, y_c) = 0$, then

- *If $|\mathbf{H}(x_c, y_c)| > 0$ and $f_{xx}(x_c, y_c) < 0$ the function has a **local maximum** at (x_c, y_c)*
- *If $|\mathbf{H}(x_c, y_c)| > 0$ and $f_{xx}(x_c, y_c) > 0$ the function has a **local minimum** at (x_c, y_c)*
- *If $|\mathbf{H}(x_c, y_c)| < 0$ the function has a **saddle point** at (x_c, y_c)*
- *If $|\mathbf{H}(x_c, y_c)| = 0$ the test is inconclusive*

A saddle point is a point where the function has a local maximum in one direction and a local minimum in another direction, like the saddle on a horse. Figure 1.34 plots the function $f(x, y) = -(x - 1)^2 + 2y^2$, which has a saddle point at $(x_c, y_c) = (1, 0)$.

EXAMPLE: Consider maximizing the function

$$f(x, y) = -(x - 1)^2 - y^2.$$

The first partial derivatives are $f_x(x, y) = -2(x - 1)$ and $f_y(x, y) = -2y$. Setting the partial derivatives to zeros and solving for x and y

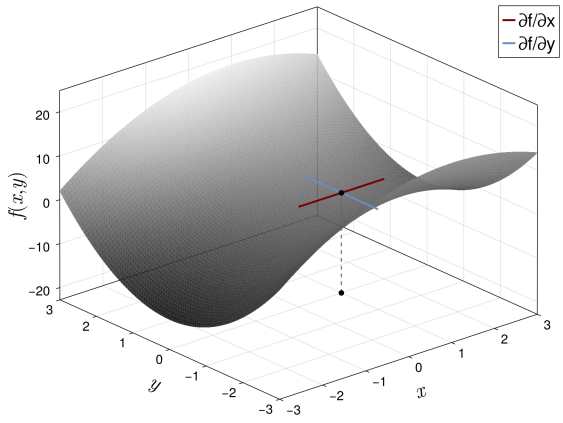

Figure 1.34: Plot of the bivariate function

$$f(x,y) = -(x-1)^2 + 2y^2$$

which has a saddle point at $(x_c, y_c) = (1,0)$. The red and blue lines are the tangent lines in the x and y directions, respectively.

gives the critical point $(x_c, y_c) = (1,0)$. The second partial derivatives are $f_{xx}(x,y) = -2$, $f_{yy}(x,y) = -2$ and $f_{xy}(x,y) = 0$. The Hessian matrix is

$$\mathbf{H}(x,y) = \begin{pmatrix} -2 & 0 \\ 0 & -2 \end{pmatrix}$$

and the determinant is $|\mathbf{H}(x,y)| = (-2)\cdot(-2) = 4 > 0$. Since $f_{xx}(x_c, y_c) < 0$, we have a local maximum at $(x_c, y_c) = (1,0)$. The function and its two partial derivatives are plotted in Figure 1.35.

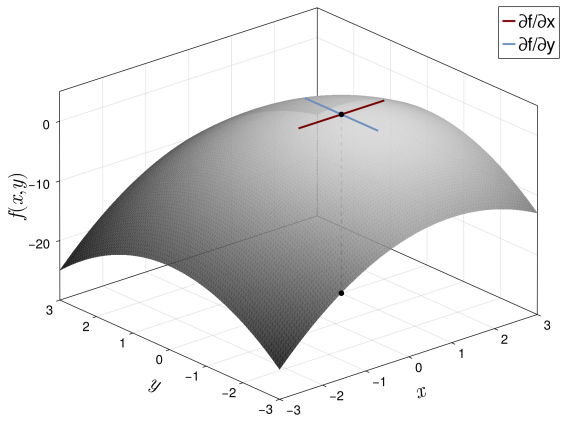

Figure 1.35: Surface plot of the function

$$f(x,y) = -(x-1)^2 - y^2$$

with its maximizer $(x_c, y_c) = (1,0)$, and the two tangent lines for the partial derivatives $f_x(x,y) = -2(x-1)$ (red line) and $f_y(x,y) = -2y$ (blue line).

All of this can be extended to functions with more than two input variables. Let $f(\mathbf{x})$ be function of n variables $\mathbf{x} = (x_1, x_2, \ldots, x_n)^\top$. The first partial derivative test finds the critical point $\mathbf{x}$ by solving the system of n equations obtained by setting the gradient vector to the zero vector

$$\frac{\partial}{\partial \mathbf{x}} f(\mathbf{x}) = (f_1(\mathbf{x}), \ldots, f_n(\mathbf{x}))^\top = \mathbf{0},$$

where $f_k(\mathbf{x}) = \frac{\partial}{\partial x_k} f(\mathbf{x})$ is the partial derivative with respect to the kth

variable. The gradient is often denoted by the symbol ∇, or $\nabla_{\mathbf{x}}$ is we want to be explicity that it is the gradient with respect to the input vector $\mathbf{x}$. It is possible to also do a second partial derivative test based on the eigenvalues of the Hessian matrix

$$\mathbf{H}(\mathbf{x}) = \frac{\partial^2}{\partial \mathbf{x} \partial \mathbf{x}^\top} f(\mathbf{x})$$

but the details are beyond the scope of this book. The Hessian is sometimes denoted by the symbol ∇^2 or $\nabla^2_{\mathbf{x}}$.

Numerical optimization using the Newton-Raphson algorithm

Many practical optimization problems are too complicated to find the maximum or minimum of a function analytically, and we need to resort to numerical algorithms. Such algorithms search for the maximum (or minimum) of a function by starting with a guess for the maximizer and then iteratively updating this guess until some stopping criteria is satisfied. There are derivative-free optimization algorithms, but we will focus on the ones that use the first and second derivatives to guide the search.

Computing the derivative $f'(x)$ of a function is usually straightforward, the hard part is to solve the equation $f'(x) = 0$ for x; this is particularly true in the case with more than one function input. The **Newton-Raphson method** is an iterative algorithm that tries to find the maximum or minimum of a twice differentiable function, i.e. a function where the first and second derivative are continuous functions of x. The basic idea is to start with an initial guess x_0 and then iteratively update the guess using the formula

Newton-Raphson method

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)} \tag{1.6}$$

where k is the iteration number. The algorithm stops when the change in x_k from one iteration to the next is smaller than some predefined tolerance ϵ, i.e. when $|x_{k+1} - x_k| < \epsilon$. Since we are searching for the x which satisfies $f'(x) = 0$, an alternative stopping criterion is to terminate the algorithm when $|f'(x_k)| < \epsilon$.

We will now explain why the Newton-Raphson update in (1.6) has that particular form. The algorithm is based on the idea that the function $f(x)$ can be approximated *locally* by a quadratic function around the current guess x_k. In Section 1.17 we learn about the Taylor approximation, which is a method for approximating a differentiable function locally around a point $x = \hat{x}$ by polynomials. The polynomials that are tailored to the function using the function's derivatives at $x = \hat{x}$. A second order Taylor approximation of $f(x)$ around the

current iteration in the Newton-Raphson algorithm is

$$f_{\text{approx}}(x_k) = f(x_k) + f'(x_k)(x - x_k) + \frac{1}{2}f''(x_k)(x - x_k)^2 \tag{1.7}$$

where $f'(x_k)$ and $f''(x_k)$ are the first and second derivatives evaluated at $x = x_k$. Now, with this quadratic approximation we can find an *approximate* maximizer using the first derivative test. Setting the first derivative of the approximation in (1.7) to zero

$$f'_{\text{approx}}(x_k) = f'(x_k) + f''(x_k)(x - x_k) = 0 \tag{1.8}$$

and solving for x gives the Newton-Raphson update x_{k+1} in (1.6).

Note that x_{k+1} is the x where the tangent line $f'_{\text{approx}}(x_k)$ crosses the horizontal line at $y = 0$. Figure 1.37 illustrates the Newton-Raphson algorithm applied to the function $f(x) = 1 + 2x^2 - (4/3)x^3$ with initial guess $x_0 = 0.7$. The larger graph plots the function $f(x)$ and marks out the maximum with a vertical dashed line. The four smaller graphs plots the derivative and each graph show a particular Newton-Raphson update. The first update at iteration 0 starts in the point $x_0 = 0.7$ and has a tangent line given by the blue line in the graph. The next iteration, x_1, is according to (1.6) where that tangent line crosses the horizontal line at $y = 0$, marked out by the vertical dashed blue line. The graph with title iteration 1 shows the following update, with tangent line in yellow leading to the new value x_2 and so on.

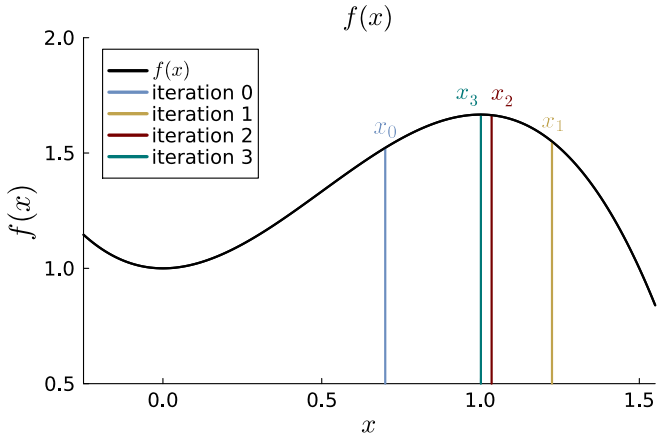

Figure 1.36: Newton-Raphson to find the maximum of the function $f(x) = 1 + 2x^2 - (4/3)x^3$ (black line) with initial value $x_0 = 0.7$. The iterations of the Newton-Raphson algorithm are plotted as vertical dashed lines.

Figure 1.36 shows the four first iterations of the Newton-Raphson algorithm applied to the function $f(x) = 1 + 2x^2 - (4/3)x^3$ with initial guess $x_0 = 0.7$. Figure 1.37 plots the derivative $f'(x) = 4x - 4x^2$ (black line) and each individual update in a separate graph with the current iteration value x_k in Newton-Raphson algorithm as a dot. The tangent lines at each iteration is plotted in the same color as the

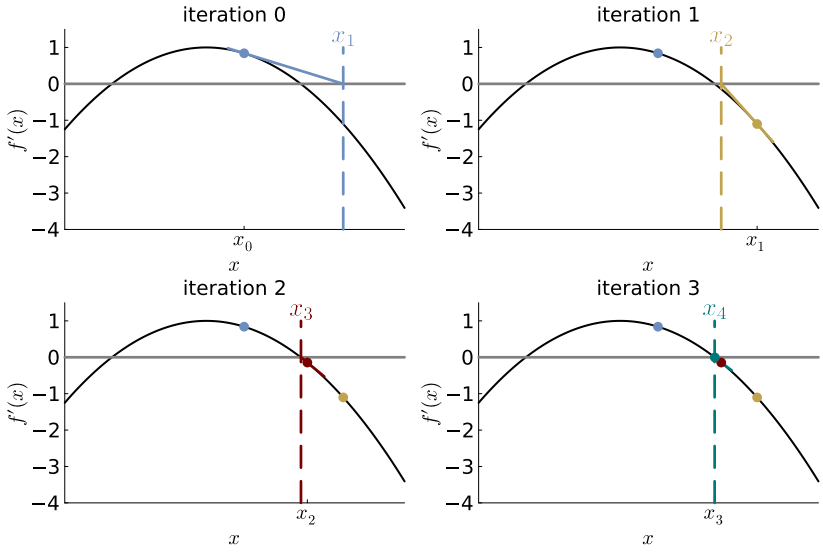

Figure 1.37: caption

current iteration and the next iteration x_{k+1} is where the tangent line crosses the gray solid horizontal line at $y = 0$. The next iteration point x_{k+1} is plotted by a vertical dashed line in the same color as the tangent line that led to it. Since the initial guess $x_0 = 0.7$ is close to the maximum, the algorithm converges quickly to the maximum at $x_{\text{max}} = 1$.

The Newton-Raphson algorithm is guaranteed to converge to a local maximum or minimum if the function is smooth and the initial guess is close enough to the optimum. If the function is actually quadratic, then the algorithm will find the optimum in one iteration. When the initial guess is far from the optimum the algorithm can take many iterations to reach the optimum. Figure 1.38 shows the convergence of the Newton-Raphson algorithm for the function $f(x) = 1 + 2x^2 - (4/3)x^3$ with three different initial values. The algorithm converges to the maximum at $x_{\text{max}} = 1$ for all three initial values, but the convergence is much faster for the initial guess $x_0 = 0.7$ than for $x_0 = 5$ and $x_0 = 20$.

In Figure 1.38 all initial values led to the same maximum, but this is not always the case. The algorithm can also converge to a local maximum or minimum that is not the global maximum or minimum. Figure 1.39 shows the Newton-Raphson algorithm applied to the same function $f(x) = 1 + 2x^2 - (4/3)x^3$ with a bad initial guess $x_0 = -0.2$. The algorithm converges to a local minimum at $x_{\text{min}} = 0$ instead of the global maximum at $x_{\text{max}} = 1$. The algorithm can also oscillate between two values or even diverge and not produce a solution at all. Repeating the algorithm several times with different

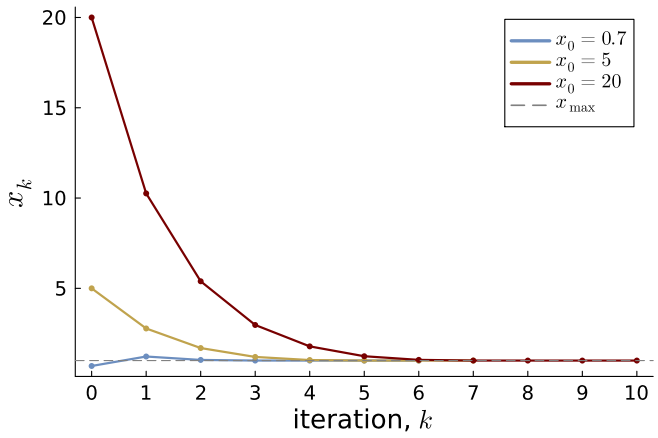

Figure 1.38: The convergence of the the Newton-Raphson algorithm for finding the maximum of the function $f(x) = 1 + 2x^2 - (4/3)x^3$ with three different initial values.

initial values and picking the solution with highest function value $f(x)$ (in case of maximization) is a recommended strategy.

The Newton-Raphson algorithm can be generalized to functions $y = f(\mathbf{x})$ with more than one variable. The update formula is then

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{H}^{-1}(\mathbf{x}_k)\nabla f(\mathbf{x}_k)$$

where $\nabla f(\mathbf{x}_k)$ is the gradient vector of first partial derivatives evaluated at $\mathbf{x}_k$ and $\mathbf{H}(\mathbf{x}_k)$ is the Hessian matrix of second partial derivatives evaluated at $\mathbf{x}_k$. The algorithm stops when the difference between two consecutive guesses is smaller than some threshold ϵ, i.e. when $||\mathbf{x}_{k+1} - \mathbf{x}_k|| < \epsilon$, where $||\cdot||$ is now the Euclidean norm of a vector (i.e. square root of sum of squared elements of the gradient).

Figure 1.40 gives Newton's method in algorithmic form, using the stopping criteria based on the value of the gradient, $|f'(\mathbf{x}_k)| < \epsilon$. The gradient vector and Hessian matrix of the function can be supplied as mathematical functions, or handled automatically by the computer using a **automatic differentiation** library. In the latter case, the user only needs to program a function that that computes the function $f(\mathbf{x})$ for any input $\mathbf{x}$ in the domain.

automatic differentiation

The inversion of the Hessian matrix can be computationally expensive, especially when $\mathbf{x}$ is high-dimensional. To save computations, **quasi-Newton** methods approximates the inverse Hessian matrix directly without ever performing the costly matrix inverse. The Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm is a popular quasi-Newton method that builds up an approximation of the inverse Hessian matrix during the iterations of the algorithm from past evaluated gradient vectors.

quasi-Newton

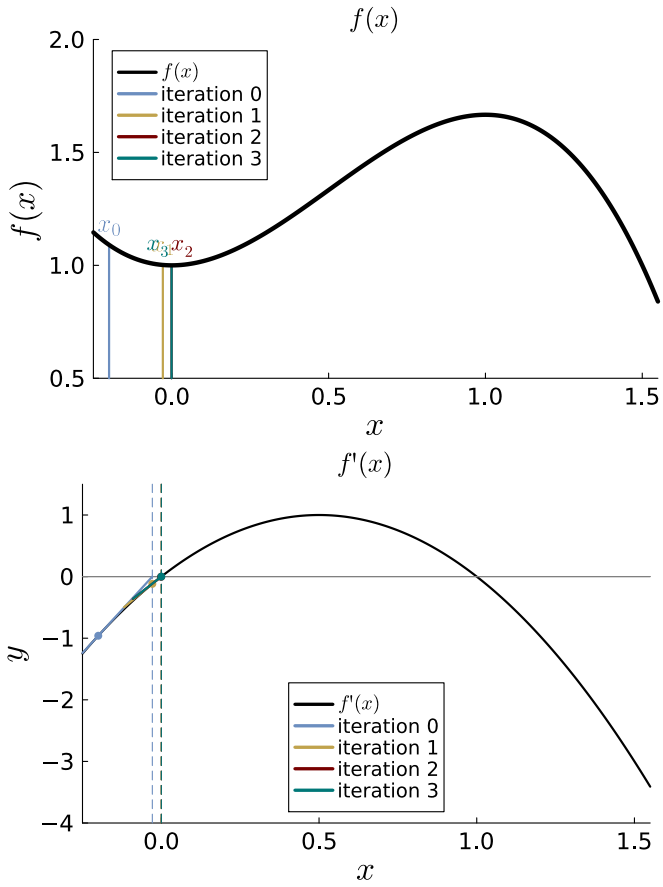

Figure 1.39: Newton-Raphson to find the maximum of the function $f(x) = 1 + 2x^2 - (4/3)x^3$ with the bad initial value $x_0 = -0.2$ that instead leads to minimum. The upper graph plots the function $f(x)$ (black line) and the iterations of the Newton-Raphson algorithm as vertical lines. The lower graph plots the derivative $f'(x) = 4x - 4x^2$ (black line), the current iteration values x_k as dots with tangent lines. The next iteration x_{k+1}, indicated by a vertical dashed line, is where the tangent line crosses the gray solid horizontal line at $y = 0$.

Newton-Raphson's method for maximizing $f(\mathbf{x})$

Input: initial guess $\mathbf{x}$
tolerance $\epsilon > 0$
while $|\nabla f(\mathbf{x})| \geq \epsilon$ **do**
  $\mathbf{x} \leftarrow \mathbf{x} - (\nabla^2 f(\mathbf{x}))^{-1} \nabla f(\mathbf{x})$
end
Output: optimizer $\mathbf{x} = \arg\max_{\mathbf{x}} f(\mathbf{x})$.

Figure 1.40: The Newton-Raphson method for finding the optimizer $\arg\max_{\mathbf{x}} f(\mathbf{x})$ of the twice differentiable function $f(\mathbf{x})$ with gradient vector $\nabla f(\mathbf{x}) = \frac{\partial}{\partial \mathbf{x}}$ and Hessian matrix $\nabla^2 f(\mathbf{x}) = \frac{\partial^2}{\partial \mathbf{x} \mathbf{x}^\top} f(\mathbf{x})$.

Numerical optimization using the gradient ascent algorithm

The Newton-Raphson algorithm requires that the first and second derivate are available. A simpler numerical maximization algorithm that only uses the first derivative is the *gradient ascent* algorithm. The idea behind the algorithm is that since the first derivative $f'(x)$ gives the slope of the function at x. If the slope is positive $f'(x_k) > 0$ at some x_k, then we can increase the function value $f(x)$ by taking the step $x_k \to x_k + \gamma \cdot f'(x_k)$ for some step size $\gamma > 0$. The step size $\gamma > 0$ should be large enough so that we take sizeable steps, but not too large since then we overshoot the target. Similarly, when the derivative is negative $f'(x_k) < 0$ we decrease x by adding the (now negative) derivative. The **gradient ascent** algorithm starts with an initial guess x_0 and then iteratively updates the guess using the formula

gradient ascent

$$x_{k+1} = x_k + \gamma \cdot f'(x_k) \tag{1.9}$$

where $\gamma > 0$ is the **step size** or **learning rate**. The algorithm stops when the derivative is smaller than some predefined tolerance ϵ, i.e. when $|f'(x_k)| < \epsilon$, or when the change in x_k from one iteration to the next is smaller than some tolerance ϵ. The gradient ascent algorithm is summarized in algorithmic form in Figure 1.43.

step size

learning rate

When the objective is to *minimize a function*, we instead subtract the derivative from the current guess, i.e. we have the update formula

$$x_{k+1} = x_k - \gamma \cdot f'(x_k)$$

This is called the **gradient descent** algorithm.

gradient descent

Figure 1.41 illustrates the gradient ascent algorithm to find the maximizer of the function $f(x) = 1 + 2x^2 - (4/3)x^3$ from an initial value of $x_0 = 0.7$. The top graph uses a suitable learning rate of $\gamma = 0.2$, giving large enough steps $\gamma \cdot f'(x_k)$ to swiftly move toward the maximum, but not too large steps that may overshot the maximum. The learning rate in the middle graph is too small, with the algorithm only slowly reaching a maximum. The bottom graph uses a too large learning rate and the algorithm ends up overshooting the maximum in every iteration. Figure 1.42 investigates the convergence of the gradient ascent algorithm with these three learning rates.

The gradient ascent algorithm can be directly generalized to functions with more than one variable. The update formula is then

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \gamma \cdot \nabla f(\mathbf{x}_k)$$

where $\nabla f(\mathbf{x}_k)$ is the gradient vector of first partial derivatives evaluated at $\mathbf{x}_k$.

The gradient ascent algorithm can be viewed as a special case of the Newton-Raphson algorithm where the inverse Hessian $H^{-1}(\mathbf{x}_k)$

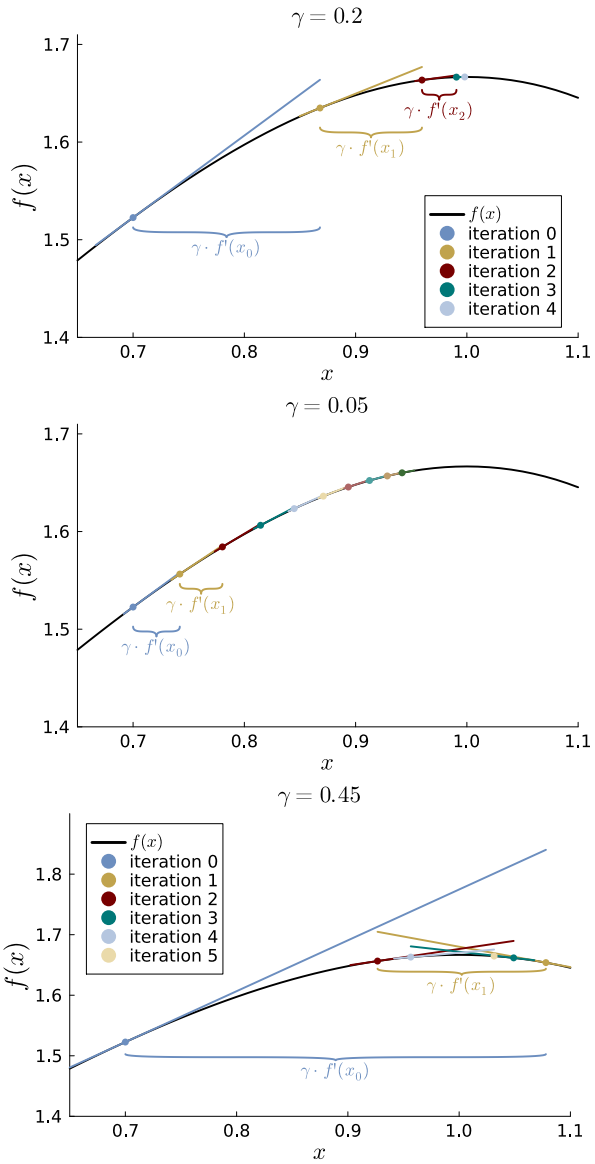

Figure 1.41: The gradient ascent algorithm for maximizing the function $f(x) = 1 + 2x^2 - (4/3)x^3$ with initial value $x_0 = 0.7$. The plots zooms in on the area around the maximum for visibility. The top graph has suitable learning rate $\gamma = 0.2$ and the algorithm approaches the maximum fairly quickly. The learning rate in the middle graph is too small, and the learning rate in the bottom graph is too large and the algorithm overshoots the maximum in each iteration.

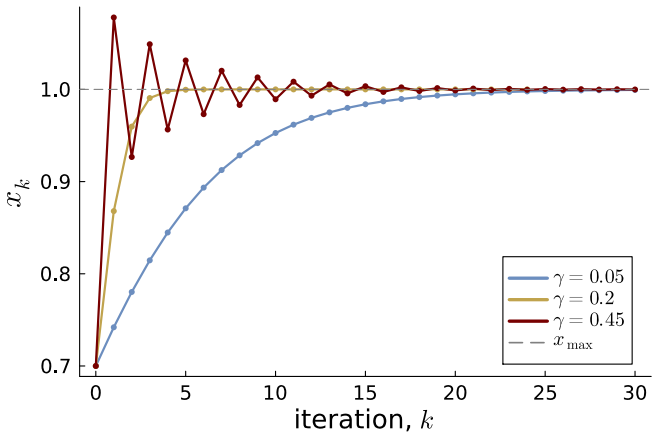

Figure 1.42: The convergence of the the gradient ascent algorithm for finding the maximum $x_{\max} = 1$ of the function $f(x) = 1 + 2x^2 - (4/3)x^3$ with three different learning rates γ. The algorithm starts with an initial guess $x_0 = 0.7$.

is replaced by $\gamma \cdot \mathbf{I}$, a diagonal matrix with the learning rate in each position on the diagonal. This means that the Newton-Raphson algorithm makes use of the geometry of the the function that we are aiming to maximize, in particular the second partial derivatives that measure the curvature of the function. This gives an adaptive step size with large steps where function is relatively flat (second partial derivatives are close to zero and inverse Hessian is therefore large) and small steps where function has a lot of curvature (large absolute value of the second partial derivatives). The simple gradient ascent algorithm is forced to use the same learning rate for all inputs and over all iterations. The gradient ascent algorithm is however more robust than the Newton-Raphson algorithms, particularly when the function is far from quadratic, and there have been a large number of clever modification of the gradient ascent algorithm that makes more use of the geometry of the optimized function.

Finally, when the gradient is very costly compute one can replace the gradient with a computationally cheaper *estimate* of the gradient, giving the **stochastic gradient ascent** algorithm used when fitting large-scale deep neural networks. The estimate of the gradient is naturally obtained by computing the gradient on a small batch of randomly selected data observations. The algorithm will nevertheless converge to the maximum if the learning rates are properly chosen and the estimate of the gradient is *unbiased* for the true gradient; see Chapter Likelihood inference for a definition of an unbiased estimator.

stochastic gradient ascent

EXERCISES

Gradient ascent algorithm for maximizing $f(\mathbf{x})$

Input: initial guess $\mathbf{x}$
tolerance $\epsilon > 0$
learning rate $\gamma > 0$
while $|\nabla f(\mathbf{x})| \geq \epsilon$ **do**
  $\mathbf{x} \leftarrow \mathbf{x} + \gamma \cdot \nabla f(\mathbf{x})$
end
Output: optimizer $\mathbf{x} = \arg\max_{\mathbf{x}} f(\mathbf{x})$.

Figure 1.43: The gradient ascent algorithm for finding the optimizer $\arg\max_{\mathbf{x}} f(\mathbf{x})$ of the differentiable function $f(\mathbf{x})$ with gradient vector $\nabla f(\mathbf{x})$.

Function optimization

1. Find the maximum of $f(x) = 1 - 3(x+1)^2$ over $x \in \mathbb{R}$ using the first derivative test. Verify that this is indeed a maximum.
2. The probability density function of the Gamma distribution is

$$p(x) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} \exp(-\beta x) \quad \text{for } x > 0,$$

where $\alpha > 0$ and $\beta >$ are constant parameters of the distribution. Find the mode of the Gamma distribution, i.e. the maximizer of $p(x)$.
[*hint*: the maximizer of $\ln p(x)$ is also the maximizer of $p(x)$.]

1.16 *Integration*

Rectangle sum approximation of areas and the integral

Integration is used to calculate **areas under functions**, as illustrated in Figure 1.45. As we will see in Chapter Probability, this is a crucial mathematical technique used for computing probabilities in statistics. Since the area under a nonlinear function can be rather non-regular, we need a clever way to do this. The basic idea is to approximate the area under a function by many small rectangles, see Figure 1.46. The area of a rectangle with base b and height h is of course $b \cdot h$; see Figure 1.44.

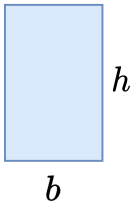

Figure 1.44: The area of a rectangle with base b and height h is $b \cdot h$.

The mathematical formulation of the rectangle approximation of the area under a function $f(x)$ between $x = a$ and $x = b$ is

$$\sum_{i=1}^{n} f(x_i^\star)\Delta x_i$$

where

$$x_0 = a < x_1 < x_2 < \ldots < x_{n-1} < x_n = b$$

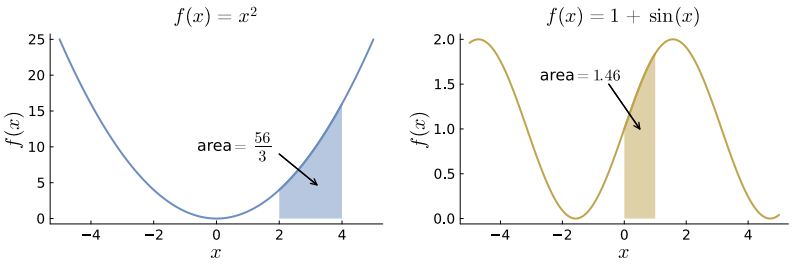

Figure 1.45: Area under the quadratic function $f(x) = x^2$ between $x = 2$ and $x = 4$ (left) and under the function $f(x) = 1 + \sin(x)$ over the interval $(0, 1)$.

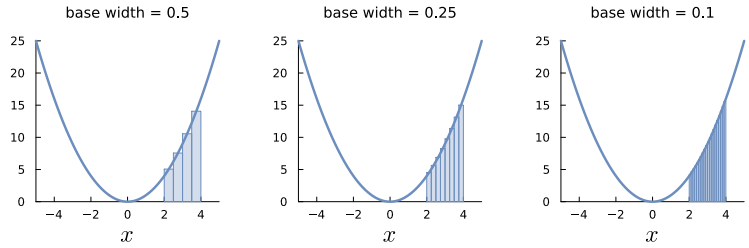

Figure 1.46: Area under the quadratic function $f(x) = x^2$ between $x = 2$ and $x = 4$ approximated with the areas of rectangles with different base widths.

is a **grid** of x-values that forms a **partition** of the interval $[a, b]$ into n bins of width $\Delta x_i = x_i - x_{i-1}$, the bases of the rectangles. The function value $f(x_i^\star)$ is the height of the ith rectangle, where $x_i^\star$ is some x-value in the ith bin. Figure 1.46 used equally sized bins with $x_i^\star$ as the midpoint between the two grid points x_{i-1} and x_i. Figure 1.47 shows some variants of the rectangle sum with each rectangle height set to the lowest function value over the bin (the *lower rectangle sum*) and the highest function values over the bin (the *upper rectangle sum*); finally, the rightmost graph in Figure 1.47 displays a rectangle sum with varying bin widths and the heights given by the midpoint rule.

partition

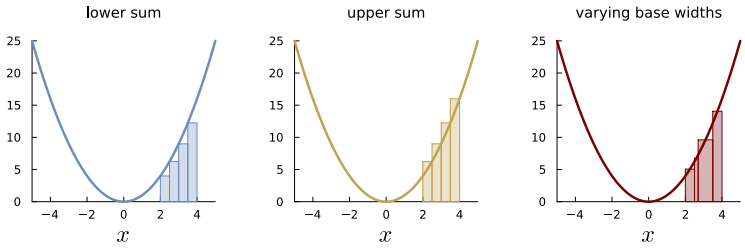

Figure 1.47: Area under the quadratic function $f(x) = x^2$ between $x = 2$ and $x = 4$ approximated with a rectangle sum with height equal to lowest value in each bin (left), highest value in each bin (middle) and with rectangles with varying widths (right).

The **Riemann integral** of a function $f(x)$ over the interval $[a, b]$ can loosely be defined as the limit of the rectangle sum

$$\sum_{i=1}^{n} f(x_i^\star)\Delta x_i$$

as the width of the rectangles approaches zero. The exact definition of the Riemann integral is a bit more complicated, and considers both the lower and upper rectangle sums in Figure 1.47 (left and middle

graph) over *all* possible partitions of the interval $[a, b]$ into rectangles, even those with varying widths (as in the right graph of Figure 1.47). The function $f(x)$ is said to be **Riemann integrable** over the interval $[a, b]$ if the lower and upper rectangle sums converge to the same limiting value as the width of the rectangles approaches zero; see Figure 1.48. That limiting value is then the (definite) **Riemann integral** of a function $f(x)$ and is denoted by

Riemann integrable

Riemann integral

$$\int_a^b f(x)\mathrm{d}x. \tag{1.10}$$

In the context of the integral in (1.10), the function $f(x)$ is called the **integrand**. The symbols a and b are called the **limits of integration**, with a being the *lower limit* and b being the *upper limit*.

integrand

limits of integration

This notation for the integral in (1.10) was not chosen without care. The integration symbol $\int$ looks like the letter s for the word *sum* and the differential symbol $\mathrm{d}x$ represents a really small version of the rectangle width Δx, approaching zero, similar to its use in the derivative. So this notation agrees with the integral as a limiting sum of rectangle areas

$$\sum_{i=1}^{n} f(x_i^\star)\Delta x_i \to \int_a^b f(x)\mathrm{d}x \quad \text{as all } \Delta x_i \to 0.$$

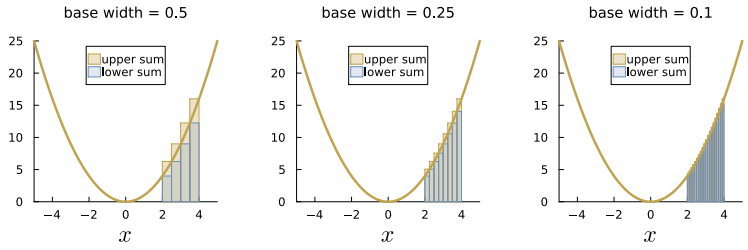

Figure 1.48: Area under the quadratic function $f(x) = x^2$ between $x = 2$ and $x = 4$ approximated with both a lower and upper rectangle sum for different base widths.

For functions $f(x)$ that can be negative, for example x^3 or $\sin(x)$, the integral can be negative. It may seem a little strange to have a negative area, but that is how the Riemann integral is defined. Figure 1.49 illustrates that areas under the function where the function is negative (blue area) contributes negatively to the total area. The integral of $\sin(x)$ from $x = -2$ to $x = 2$ is the sum of the positive area (yellow) and the negative area (blue), giving a total integral of zero.

Anti-derivatives and rules for integration

It would be a nightmare is we had to take the limit of the Riemann sum every time we want to integrate a function. Luckily there is a much simpler route using something called the **anti-derivative** of a function. The anti-derivative is also called the **indefinite integral** and

anti-derivative

indefinite integral

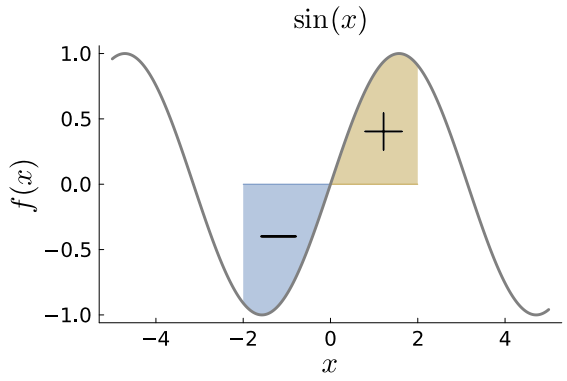

Figure 1.49: Area under the function where the function is negative contributes negatively to the total area.

can be seen as the reverse operation of differentiation. Here is the definition.

Definition. *A function $F(x)$ is the **anti-derivative** to the function $f(x)$ if*

$$F'(x) = \frac{\mathrm{d}}{\mathrm{d}x}F(x) = f(x), \text{ for all } x$$

Figure 1.50 gives anti-derivatives of some common elementary functions.

The anti-derivative can also be written in an alternative notation using the integral sign without limits of integration:

$$F(x) = \int f(x)\mathrm{d}x.$$

The definite integral $\int_a^b f(x)\mathrm{d}x$ is a number, the anti-derivative $F(x) = \int f(x)\mathrm{d}x$ is a function of x. Since the anti-derivative $F(x)$ to the function $f(x)$ is by definition a function whose derivative is $f(x)$, we can write

$$\frac{\mathrm{d}}{\mathrm{d}x}\underbrace{\int f(x)\,\mathrm{d}x}_{F(x)} = f(x)$$

which clearly shows that integration is the reverse operation of differentiation.

Anti-derivatives are life-savers when it comes to integration since they can be used to compute definite integrals, as the following **second fundamental theorem of calculus** shows.

second fundamental theorem of calculus

Theorem 3. *If $f(x)$ is integrable on $[a,b]$ and $F(x)$ is an anti-derivative of $f(x)$, then*

$$\int_a^b f(x)\mathrm{d}x = F(b) - F(a),$$

It is often convenient to use the notation $[F(x)]_a^b$ for $F(b) - F(a)$ as it allows us to first express the anti-derivative as a function of x and then in a second step evaluate $F(x)$ at the two interval endpoints a and b. Here is an example to illustrate this point.

EXAMPLE: Let us integrate the function $f(x) = x^2$ from $a = 1$ to $b = 3$, see Figure X. The anti-derivative $F(x)$ is the function whose derivative is $f(x) = x^2$. We know that $\frac{d}{dx}x^3 = 3x^2$, so an anti-derivative to x^2 is $F(x) = \frac{1}{3}x^3$; let us check to be sure: by the power rule $F'(x) = 3\frac{1}{3}x^2 = x^2 = f(x)$, so it checks out. However, since additive constants have derivative zero, the function $F(x) = \frac{1}{3}x^3 + C$ for *any* constant C is also an anti-derivative to $f(x) = x^2$. The constant C will cancel out when computing the definite integral, so we can safely ignore it here. By the second fundamental theorem of calculus we have therefore have

$$\int_1^3 x^2 \,\mathrm{d}x = \left[\frac{1}{3}x^3\right]_1^3 = \frac{3^3}{3} - \frac{1^3}{3} = 9 - \frac{1}{3} = 8\frac{2}{3}.$$

Note the convenience in the bracket notation $[F(x)]_a^b = \left[\frac{1}{3}x^3\right]_1^3$.

Anti-derivatives of elementary functions

$f(x)$	$F(x)$	comment
x^n	$\frac{1}{n+1}x^{n+1}$	for $n \neq -1$
e^{ax}	$\frac{1}{a}e^{ax}$	for $a \neq 0$
$\frac{1}{x}$	$\ln \lvert x \rvert$	
a^x	$\frac{a^x}{\ln a}$	
$\sin x$	$-\cos x$	
$\cos x$	$\sin x$	

Figure 1.50: Integrals of common elementary functions. The constant of integration C is ignored here.

The anti-derivatives to many common functions are known; see Figure 1.50 for some of these results. Also, similar to differentiation, there are rules for the integral of a sum or a product of two or more functions; see Figure 1.51. For example, the integral of a sum of functions is the sum of the integrals of the functions.

$$\int_a^b \big(f(x) + g(x)\big)\,\mathrm{d}x = \int_a^b f(x)\,\mathrm{d}x + \int_a^b g(x)\,\mathrm{d}x.$$

The product rule for integration

$$\int_a^b f(x)g'(x)\,\mathrm{d}x = \big[f(x)g(x)\big]_a^b - \int_a^b f'(x)g(x)\,\mathrm{d}x$$

is usually called *integration by parts* and is the reverse of the product rule for differentiation. Note however that while the left hand side of the product rule is the integral of two functions, the second function in the product is the derivative of $g(x)$. We illustrate the mechanics of integration by parts in the following example.

Integrals for combinations of functions

Constant rule	$\int_a^b kf(x)\,\mathrm{d}x = k\int_a^b f(x)\,\mathrm{d}x$ for constant k
Sum rule	$\int_a^b \big(f(x)+g(x)\big)\,\mathrm{d}x = \int_a^b f(x)\,\mathrm{d}x + \int_a^b g(x)\,\mathrm{d}x$
Product rule	$\int_a^b f(x)g'(x)\,\mathrm{d}x = \big[f(x)g(x)\big]_a^b - \int_a^b f'(x)g(x)\,\mathrm{d}x$

Figure 1.51: Integrals of sums and products of two integrable functions $f(x)$ and $g(x)$. The product rule is often called integration by parts.

EXAMPLE: Let us compute the integral of the function $3x^2 + e^x$ from $a = 1$ to $b = 2$. Using the sum rule for integration we can split the integral into two parts:

$$\int_1^2 (3x^2 + e^x)\,\mathrm{d}x = \int_1^2 3x^2\,\mathrm{d}x + \int_1^2 e^x\,\mathrm{d}x.$$

The first integral can be computed using the constant rule from Figure 1.51followed by the anti-derivative for power functions in Figure 1.50, which gives

$$\int_1^2 3x^2\,\mathrm{d}x \overset{\text{constant}}{=} 3\int_1^2 x^2\,\mathrm{d}x \overset{\text{power}}{=} 3\Big[\frac{1}{3}x^3\Big]_1^2 = \Big[x^3\Big]_1^2 = 8 - 1 = 7.$$

The second integral can be computed using the anti-derivative of e^x, which is e^x itself, so we have

$$\int_1^2 e^x\,\mathrm{d}x = \Big[e^x\Big]_1^2 = e^2 - e^1.$$

Putting it all together we have

$$\int_1^2 (3x^2 + e^x)\,\mathrm{d}x = 7 + (e^2 - e^1) \approx 11.671.$$

EXAMPLE: Let us compute the integral of the function xe^x from $a = 1$ to $b = 2$. Here we identify $f(x) = x$ and $g'(x) = e^x$, where the anti-derivative to $g'(x)$ is $g(x) = e^x$ since $\frac{\mathrm{d}}{\mathrm{d}x}e^x = e^x$. The product rule for integration now says that

$$\int_1^2 xe^x\,\mathrm{d}x = \big[xe^x\big]_1^2 - \int_1^2 1\cdot e^x\,\mathrm{d}x,$$

since $\frac{\mathrm{d}}{\mathrm{d}x}x = 1$. The first term above is $\left[xe^x\right]_1^2 = 2e^2 - e^1$. The second term is $\int_1^2 e^x = [e^x]_1^2 = e^2 - e^1$. Hence the integral is

$$\int_1^2 xe^x \,\mathrm{d}x = (2e^2 - e^1) - (e^2 - e^1) = e^2 \approx 7.38906.$$

Note that for the integration by parts formula to be useful we must be able to compute the integral $\int_a^b f'(x)g(x)$, which was possible above due to the simple form of $f'(x) = 1$ in this example. Put differently, integration by parts replaces one integral $\int_a^b f(x)g'(x)$ with another integral $\int_a^b f'(x)g(x)$, with the hope that the latter integral is easier to compute than the former. We can freely choose which function plays the role of $f(x)$ and which plays the role of $g'(x)$ in the product rule, to make the problem more easy to solve.

Improper integrals

So far we have implicitly only considered the case where

- the integrand $f(x)$ in the integral $\int_a^b f(x)\mathrm{d}x$ is bounded, i.e. when all function values $f(x)$ are finite (not $-\infty$ or ∞) for all x in the interval $[a, b]$, and
- the interval boundaries a and b are both finite.

It is however common to have integration problems where one or even both of these restriction do not hold; an integral of this type is called an **improper integral**. As we will see in the Chapter Probability, we often want to compute probabilities of the form $\Pr(X \leq b)$ for some constant b, which corresponds to the integrals of the form $\int_{-\infty}^b f(x)\mathrm{d}x$, where $f(x)$ is the so called probability density function; here the lower interval boundary a is $-\infty$. We will only discuss the second case with infinite interval boundaries, but the first case with unbounded integrand is treated in a similar way.

improper integral

The integral in the cases with $a = -\infty$, $b = \infty$ or both $a = -\infty$ and $b = \infty$ is handled using a two-step approach where:

- we first compute the integral $\int_a^b f(x)\mathrm{d}x$ for some finite a and b
- then take the limit of that integral as $a \to -\infty$:

$$\int_{-\infty}^b f(x)\mathrm{d}x = \lim_{a\to-\infty} \int_a^b f(x)\mathrm{d}x$$

Similarly for the case where the upper interval boundary b is infinite, the integral is defined as $\int_a^b f(x)\mathrm{d}x$ for finite b and then taking the limit as $b \to \infty$:

$$\int_a^\infty f(x)\mathrm{d}x = \lim_{b\to\infty} \int_a^b f(x)\mathrm{d}x$$

As with any limit, these limits may or may not exist. If the limit exists, the integral is said to be **convergent**, otherwise it is **divergent**. Here are two examples, one divergent and one convergent.

convergent

divergent

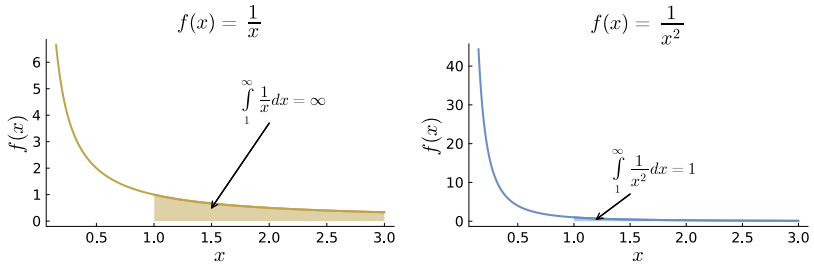

Figure 1.52: Illustration of the divergent integral of the function $f(x) = \frac{1}{x}$ from $x = 1$ to $x = \infty$ (left) and the convergent integral of the function $f(x) = \frac{1}{x^2}$ from $x = 1$ to $x = \infty$ (right).

EXAMPLE: The integral of the function $f(x) = \frac{1}{x}$ from $a = 1$ to $b = \infty$ is

$$\int_1^\infty \frac{1}{x} \mathrm{d}x = \lim_{b\to\infty} \int_1^b \frac{1}{x} \mathrm{d}x = \lim_{b\to\infty} \Big[\ln x \Big]_1^b = \lim_{b\to\infty} (\ln b - \ln 1) = \infty,$$

where we used that $\ln(|x|)$ is an anti-derivative to $1/x$ (see Figure 1.50) and x is always positive over the interval of integration so we can get rid of the absolute value sign (since $|x| = x$ for $x > 0$). The integral is divergent since the integral grows without bound as the upper limit b approaches infinity. The integral diverges because the function $f(x) = \frac{1}{x}$ decays to zero too slowly as $x \to$; see the left graph in Figure 1.52; even though the area seems to be finite in the figure, the area of the function over the region $x > 3$ not shown in the graph is actually infinitely large.

EXAMPLE: Suppose now that we want to compute the integral of the function $f(x) = \frac{1}{x^2}$ over the same interval $[1, \infty]$. The integral is

$$\int_1^\infty \frac{1}{x^2} \mathrm{d}x = \lim_{b\to\infty} \int_1^b \frac{1}{x^2} \mathrm{d}x = \lim_{b\to\infty} \Big[-\frac{1}{x} \Big]_1^b = \lim_{b\to\infty} \Big(-\frac{1}{b} - \Big(-\frac{1}{1} \Big) \Big) = 1,$$

since $\lim_{b\to\infty} \frac{1}{b} = 0$. The integral converges to a finite value as the upper limit b approaches infinity; it is convergent. The function $f(x) = \frac{1}{x^2}$ decays to zero sufficiently fast as $x \to \infty$ for the integral to be convergent; see the right graph of Figure 1.52.

Integration with multiple input variables

In statistics we are often interested in *joint* probabilities for two random variables X and Y; for example the probability that X is in some interval (a, b) *and* Y in some interval (c, d):

$$\Pr(a \leq X \leq b, c \leq Y \leq d).$$

Chapter Joint distributions shows that computing such joint probabilities involves integration of functions with two input variables, $f(x, y)$.

For a function $f(x)$ with a single input x, the *integral* $\int_a^b f(x)\,\mathrm{d}x$ calculates the *area under the curve* defined by the function $f(x)$ over the interval (a, b); see the left graph of Figure 1.53 for a reminder. The *double integral* for functions $f(x, y)$ with two inputs x and y computes the *volume under the surface* defined by the function $f(x, y)$ over some region in the two-dimensional input space (x, y); a surface in 3D space is like a sheet. The right graph of Figure 1.53 illustrates the double integral of $f(x, y) = x^2 \exp(y)$ over the square region $(x, y) \in [0, 2] \times [0, 2]$. The region of integration is marked out by a black rectangle in (x, y)-space, and the volume under the surface is represented by the darker shaded area in the figure.

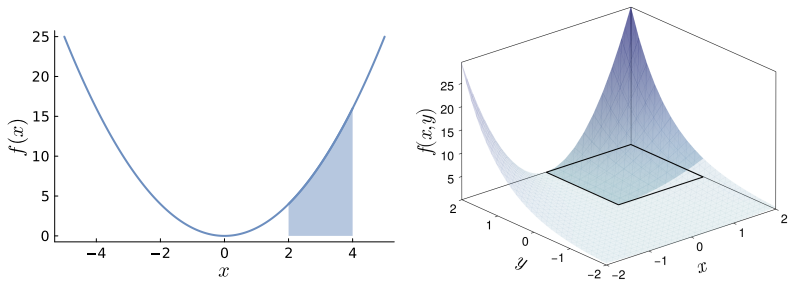

Figure 1.53: The single integral $\int_a^b f(x)\,\mathrm{d}x$ of a function $f(x)$ calculates the area under the curve (left), while the double integral $\int_c^d \int_a^b f(x, y)\,\mathrm{d}x\,\mathrm{d}y$ of a two-dimensional function $f(x, y)$ calculates the volume under the surface.

The idea of approximating an area by a rectangle sum in the case with one input is now replaced by approximating the volume under the function surface by a rectangle cuboid sum. A *rectangle cubiod* is a three-dimensional rectangle; see Figure 1.54. Basic geometry tells us that the area of a rectangle cuboid is $b_x \cdot b_y \cdot h$, where b_x is the base along the x-axis, b_y is the base along the y-axis and h is the height of the cuboid. Figure 1.56 illustrates the idea of approximating volume with sums of rectangle cuboids. The left graph shows the approximation with a few cuboids, while the right graph shows the approximation with many cuboids. The more cuboids we use, the better the approximation of the volume under the surface.

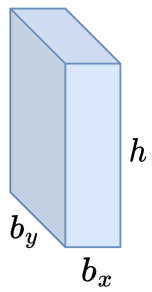

Figure 1.54: The area of a rectangular cuboid is $b_x \cdot b_y \cdot h$.

Define a partition of the x-axis into m bins, $a = x_0 < x_1, \ldots, x_m = b$, and similarly for the y-axis into n bins, $c = y_0 < y_1, \ldots, y_n = d$. The rectangle cuboid sum approximation of the integral of $f(x, y)$ over the region $(a, b) \times (c, d)$ is then given by

$$\sum_{j=1}^{n} \sum_{i=1}^{m} f(x_i^\star, y_j^\star) \Delta x_i \Delta y_j$$

Δx_i and Δy_j are the two bases of the cuboid containing the point

$(x_i^\star, y_j^\star)$ and the height of the cuboid is $f(x_i^\star, y_j^\star)$. See Figure for an illustration. The double sum above can be replaced by a single sum with $m \cdot n$ terms; the important part is that we sum the volumes of all $m \cdot n$ rectangle cubiods; see Figure 1.56.

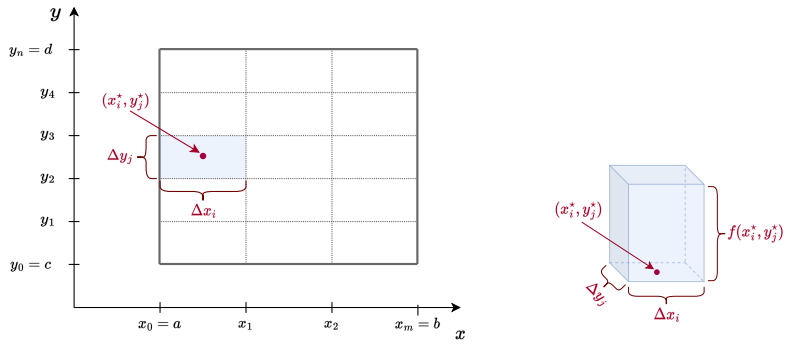

Figure 1.55: Illustration of the partition of the x-axis into m bins, $a = x_0 < x_1, \ldots, x_m = b$, and the y-axis into n bins, $c = y_0 < y_1, \ldots, y_n = d$ making up a total of $m \cdot n$ rectangles in the (x, y)-space, which forms the base of the rectangle cuboids used to approximate the volume under the surface.

Similar to the development of the Riemann integral in one dimension, the **double integral** of $f(x, y)$ is now the limit of the rectangle cuboid sum as both $\Delta x_i \to 0$ and $\Delta y_i \to 0$. Since the rectangle cuboid sum is a double sum, the following notation is quite natural for the double integral

double integral

$$\int_c^d \int_a^b f(x, y) \, \mathrm{d}x \, \mathrm{d}y$$

This is the *definite* double integral. Note that the inner integral $\int_a^b$ is with respect to x and the outer integral $\int_c^d$ is with respect to y. To make this more clear, we can write the double integral as

$$\int_{y=c}^{y=d} \int_{x=a}^{x=b} f(x, y) \, \mathrm{d}x \, \mathrm{d}y.$$

An *indefinite* double integral is written

$$\iint f(x, y) \, \mathrm{d}x \, \mathrm{d}y.$$

As in the case with a single variable, the definite integral is an number while the indefinite integral is a function of both x and y.

Example: Let us compute the double integral of the function $f(x, y) = xy$ over the rectangle $(x, y) \in (0, 1) \times (0, 1)$, i.e. $a = 0$, $b = 1$, $c = 0$ and $d = 1$. In this case we can integrate the function $f(x, y)$ in two steps:

1. first integrate with respect to x **while treating** y **as a constant**
2. then integrate with respect to y.

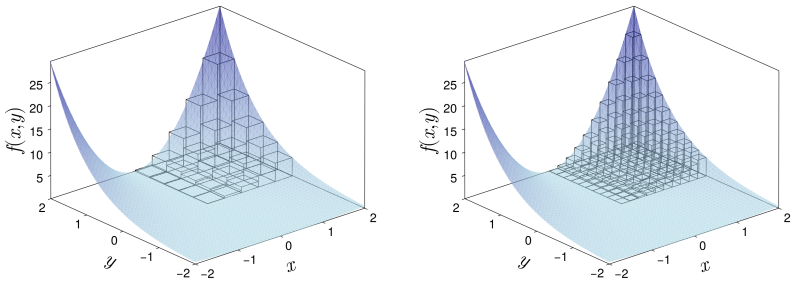

Figure 1.56: Rectangular cuboid sum approximation of the integral of $f(x,y) = x^2 \exp(y)$ over the region $(x,y) \in (0,2) \times (0,2)$ with $n_x \cdot n_y = 5 \cdot 5 = 25$ cuboids (left) and $n_x \cdot n_y = 10 \cdot 10 = 100$ cuboids (right).

We can also do the opposite, i.e. integrate with respect to y first while treating x as a constant, and then integrate with respect to x. The order of integration does not matter. To see the two steps clearly, we can write the double integral with parentheses around the first *inner integral*:

$$\int_0^1 \int_0^1 xy \, \mathrm{d}x \, \mathrm{d}y = \int_0^1 \Big(\int_0^1 xy \, \mathrm{d}x \Big) \, \mathrm{d}y.$$

The first step above is then computing this inner integral first, as a completely separate integral where y is treated like any other constant

$$\int_0^1 xy \, \mathrm{d}x = \Big[\frac{1}{2} x^2 y \Big]_0^1 = \frac{1}{2} y.$$

After that we calmly take care of the *outer integral* with respect to y:

$$\int_0^1 \frac{1}{2} y \, \mathrm{d}y = \Big[\frac{1}{4} y^2 \Big]_0^1 = \frac{1}{4}.$$

Here are the two steps performed on a single line:

$$\int_0^1 \int_0^1 xy \, \mathrm{d}x \, \mathrm{d}y = \int_0^1 \Big[\frac{1}{2} x^2 y \Big]_0^1 \mathrm{d}y = \int_0^1 \frac{1}{2} y \, \mathrm{d}y = \Big[\frac{1}{4} y^2 \Big]_0^1 = \frac{1}{4}.$$

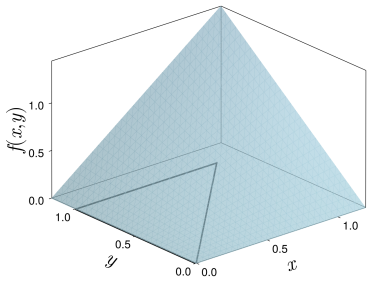

Figure 1.57: Integral of the function $f(x,y) = xy$ (blue surface) over the triangular region in $(x,y) \in (0,1) \times (0,1)$ where $x \leq y$ marked out by the black triangle in (x,y) space.

We have so far implicitly assumed that the region of integration is a rectangle in the (x,y)-space, i.e. $a \leq x \leq b$ and $c \leq y \leq d$. However, it is possible to integrate over other regions as well. For example, we can integrate the function $f(x,y) = xy$ over a triangle in (x,y)-space;

see Figure 1.57. In this case the region of integration is defined by the inequalities $0 \leq x \leq 1$ and $0 \leq y \leq 1$ and $x \leq y$. In general, we write the double integral over a region R in the (x, y)-space as

$$\iint_R f(x, y)\,\mathrm{d}x\,\mathrm{d}y$$

where R is the region of integration, for example the triangle in Figure 1.57, or something more complex. The symbol $\iint_R$ is a shorthand notation for the double integral over the region R in the (x, y)-space and the two integral signs should be read as a single double integral; the limit of integration R belongs to both integral signs, not only the second one, as the notation may suggest.

We can still perform the integral over non-rectangular regions in the two steps outlined above, but we need to be careful about the limits of integration since we now also have the restriction $x \leq y$ in addition to the $0 \leq x \leq 1$ and $0 \leq y \leq 1$. If we start with the integration of x for a constant y then the limits of integration for x is therefore $0 \leq x \leq y$, i.e. the upper limit of integration is given by the other variable y. The inner integral is then (note that the upper limit of integration is y):

$$\int_0^y xy\,\mathrm{d}x = \left[\frac{1}{2}x^2 y\right]_0^y = \frac{1}{2}y^3.$$

With the variable x out of the way (integrated out), the outer integral with respect to y has simple integration limits $0 \leq y \leq 1$:

$$\int_0^1 \frac{1}{2}y^3\,\mathrm{d}y = \left[\frac{1}{8}y^4\right]_0^1 = \frac{1}{8}.$$

Again, we can write the two steps on a single line:

$$\int_0^1 \int_0^y xy\,\mathrm{d}x\,\mathrm{d}y = \int_0^1 \left[\frac{1}{2}x^2 y\right]_0^y \mathrm{d}y = \int_0^1 \frac{1}{2}y^3\,\mathrm{d}y = \left[\frac{1}{8}y^4\right]_0^1 = \frac{1}{8}.$$

For continuous functions, the order of integration does not matter, and we can also integrate with respect to y first. In this case the limits of integration for the inner integral with respect to y is $x \leq y \leq 1$, where the lower limit of integration is given by the other variable x. The end result is the same volume $\frac{1}{8}$.

EXERCISES

Integration

1. Compute the definite integral $\int_1^2 3(x+1)^2\,\mathrm{d}x$
2. Compute the definite integral $\int_1^2 e^x\,\mathrm{d}x$

3. Compute $\int_0^5 3 \, \mathrm{d}x$
4. Compute $\int_0^3 (1.5t^2 + t) \, \mathrm{d}t$
5. Compute the indefinite integral (anti-derivative) $\int \frac{1}{y^5} \, \mathrm{d}y$
6. Compute $\int y(\frac{3}{2}y^2 + y) \, \mathrm{d}y$
7. Compute $\int_0^\infty \frac{1}{2} e^{-x/2} \, \mathrm{d}x$
8. Compute $\int_{y_1=0}^{y_1=2} e^{-y_1} \, \mathrm{d}y_1$

1.17 *Function approximation*

Approximating a function with a single input variable

The Taylor approximation is a tailored[1] polynomial approximation of a function $f(x)$. The **Taylor series** of an infinitely differentiable function $f(x)$ is

$$f(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(a)}{k!}(x-a)^k, \tag{1.15}$$

where $f^{(k)}(a)$ is the kth derivative of f evaluated in the point $x = a$.

[1] The Taylor approximation is named after the mathematician Brook Taylor. But, as we will see, it is an approximation that tailors a polynomial to the function. So, yes, an informative word play.

Taylor series

The classical example of a Taylor series is that of the exponential function. The derivatives of the exponential function $f(x) = e^x$ are the exponential function itself, i.e. $f^{(k)}(x) = e^x$ for all k. The Taylor series expansion of the exponential function around $x = 0$ is therefore

$$\begin{aligned} e^x &= e^0 + \frac{1}{1!}e^0(x-0) + \frac{1}{2!}e^0(x-0)^2 + \frac{1}{3!}e^0(x-0)^3 + \dots \\ &= 1 + \frac{x^1}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots \\ &= \sum_{k=0}^{\infty} \frac{x^k}{k!}. \end{aligned}$$

A **Taylor approximation** of $f(x)$ uses only a small number of terms in the Taylor series

Taylor approximation

$$f(x) \approx \sum_{k=0}^{K} \frac{f^{(k)}(a)}{k!}(x-a)^k, \tag{1.16}$$

for some finite and typically small K. Figure 1.58 shows how the Taylor approximation of e^x improves as higher order polynomial terms are included in the approximation. Taylor's theorem can be used to bound the approximation error of a kth order Taylor approximation using the $(k+1)$th derivative of the function.

The Taylor expansion is a local approximation around the expansion point $x = a$, and the approximation is most accurate in a neighborhood around a. This point is illustrated in Figure 1.59 where the function $\log(1+x)$ is well approximated only in the neighborhood around the expansion point $x = 0$.

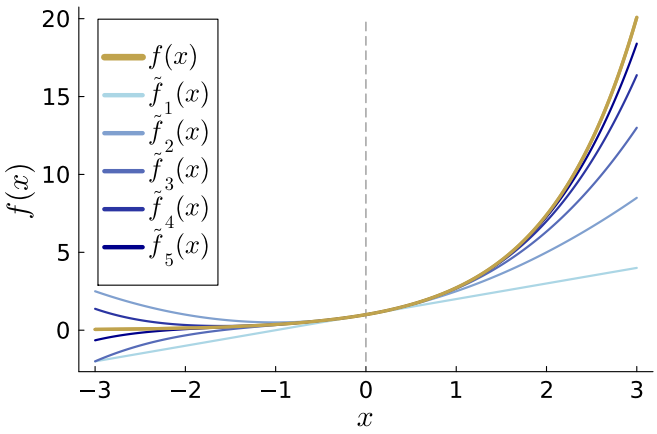

Figure 1.58: Taylor approximation of the exponential function for different polynomial orders.

In this observable widget you can see the Taylor approxmation in action for some commonly used functions; in particular, the widget lets you experiment with different polynomial orders and evaluation points a.

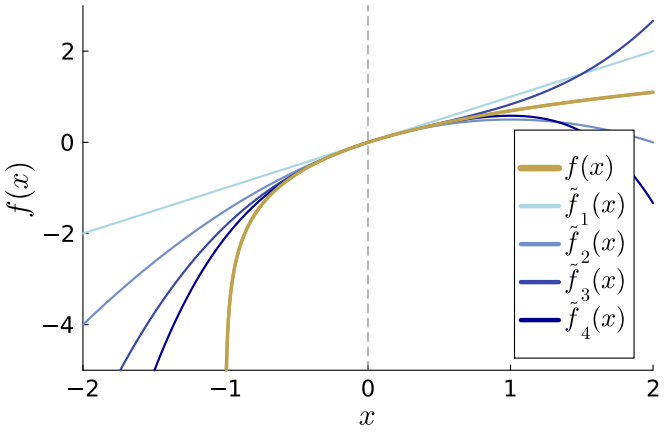

Figure 1.59: Taylor approximation of $\log(1+x)$ around $x = 0$ for different approximation orders.

Approximating a function with multiple input variables

There is a multivariable version of the Taylor approximation for functions $f(\mathbf{x}) = f(x_1, \ldots, x_d)$ of several variables. We will only make use of the first and second order versions.

The first order Taylor approximation of the function $f(\mathbf{x})$ around the point $\mathbf{x} = \mathbf{a}$ is

$$f(\mathbf{x}) \approx f(\mathbf{a}) + \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}|_{\mathbf{x}=\mathbf{a}}(\mathbf{x} - \mathbf{a}),$$

where

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

is the **gradient** row vector with partial derivatives of $f(\mathbf{x})$ with respect to each of the input variables $x_1, \ldots, x_d$. The notation $\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}|_{\mathbf{x}=\mathbf{a}}$ means that this vector of derivatives is evaluated in the point $\mathbf{x} = \mathbf{a}$. A first order Taylor approximation approximates the function $f(\mathbf{x})$ with a (hyper)plane tangent to the function at the point $\mathbf{x} = \mathbf{a}$. gradient

The second order Taylor approximation of the function $f(\mathbf{x})$ around the point $\mathbf{x} = \mathbf{a}$ is

$$f(\mathbf{x}) \approx f(\mathbf{a}) + \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}|_{\mathbf{x}=\mathbf{a}}(\mathbf{x}-\mathbf{a}) + \frac{1}{2}(\mathbf{x}-\mathbf{a})^\top \frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^\top}|_{\mathbf{x}=\mathbf{a}}(\mathbf{x}-\mathbf{a}),$$

where the $d \times d$ matrix $\frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^\top}$ is the **Hessian** matrix Hessian

$$\frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^\top} = \begin{pmatrix} \frac{\partial^2 f(\mathbf{x})}{\partial x_1^2} & \frac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_d} \\ \frac{\partial^2 f(\mathbf{x})}{\partial x_2 \partial x_1} & \frac{\partial^2 f(\mathbf{x})}{\partial x_2^2} & & \frac{\partial^2 f(\mathbf{x})}{\partial x_2 \partial x_d} \\ \vdots & & \ddots & \\ \frac{\partial^2 f(\mathbf{x})}{\partial x_d \partial x_1} & \frac{\partial^2 f(\mathbf{x})}{\partial x_d \partial x_2} & & \frac{\partial^2 f(\mathbf{x})}{\partial x_d^2}, \end{pmatrix}$$

with second derivatives $\frac{\partial^2 f(\mathbf{x})}{\partial x_j^2}$ and cross-derivatives $\frac{\partial^2 f(\mathbf{x})}{\partial x_j \partial x_k}$.

To see the multidimensional Taylor approximation in action, consider the following two-dimensional function

$$f(x_1, x_2) = \exp(x_1)\sin(x_2).$$

To compute a second order Taylor approximation around $\mathbf{x} = (0,0)^\top$ we need to compute the gradient vector and Hessian matrix. The gradient vector is

$$\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} = \Big(\exp(x_1)\sin(x_2), \exp(x_1)\cos(x_2)\Big),$$

which evaluates to $(0,1)$ at $\mathbf{x} = (0,0)^\top$. The Hessian matrix is

$$\frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^\top} = \begin{pmatrix} \exp(x_1)\sin(x_2) & \exp(x_1)\cos(x_2) \\ \exp(x_1)\cos(x_2) & -\exp(x_1)\sin(x_2) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

at $\mathbf{x} = (0,0)^\top$. The second order Taylor approximation is therefore

$$f(x_1, x_2) \approx 0 + (0,1)(x_1, x_2)^\top + \frac{1}{2}(x_1, x_2)^\top \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} (x_1, x_2) = x_2 + 2x_1x_2.$$

Figure 1.60 plots the second order Taylor approximation of $\exp(x_1)\sin(x_2)$.

EXERCISES

Function approximation

1. Some function approximation problem here.

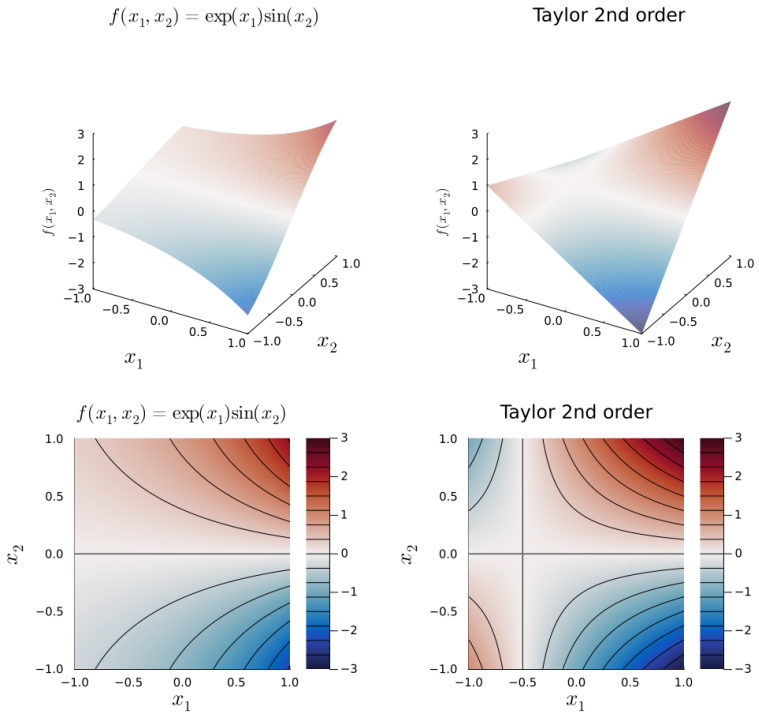

Figure 1.60: Taylor approximation of $f(x_1, x_2) = \exp(x_1)\sin(x_2)$ around $\mathbf{x} = (0, 0)$. The graphs in the first row show function surface plots and the second row displays corresponding heatmaps and contours of the functions.

1.18 *Linear algebra*

This section summarizes some selected results from matrix algebra and multivariate analysis. The results are mostly given without proof, and the reader is referred to for example Harville (1998) for an extensive account or Appendix A in Mardia et al. (1979) for a more condensed treatment. The starred sections are not required for understanding the material in the Bayesian Learning book, but are widely used results that every statistician should know about.

Vectors, matrices and their products

A **vector** vector

$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_p \end{pmatrix}$$

is a collection of real numbers. We always define vectors as *column* vectors. A vector can be turned into a row vector by the **vector transpose** $\mathbf{a}^\top = (a_1, a_2, \ldots, a_p)$. A vector can be viewed geometrically as an arrow in p-dimensional space $\mathbb{R}^p$ with p coordinates, such that a vector has a direction and a length. For example, a vector with two elements represents an arrow in the two-dimensional plane $\mathbb{R}^2$ (left

vector transpose

graph in Figure 1.61), while a vector with three elements represents an arrow in the three-dimensional space $\mathbb{R}^3$ (right graph in Figure 1.61).

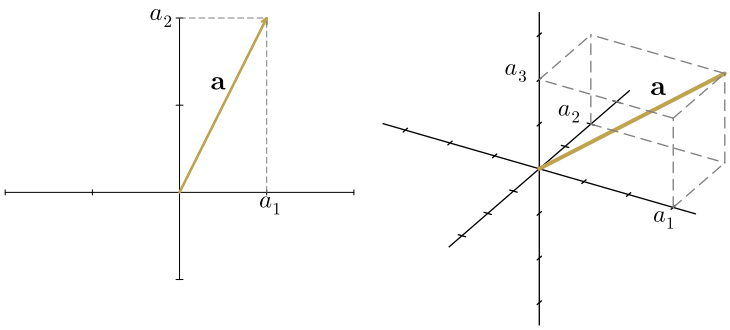

Figure 1.61: Geometric illustration of a two-element vector $\mathbf{a} = (a_1, a_2)^\top$ in $\mathbb{R}^2$ (left) and a three-element vector $\mathbf{a} = (a_1, a_2, a_3)^\top$ in $\mathbb{R}^3$.

The **dot product** of two vectors $\mathbf{a}$ and $\mathbf{b}$ with the same number elements is defined as

dot product

$$\mathbf{a}^\top \mathbf{b} = \sum_{j=1}^{p} a_j b_j,$$

which is often written as $\mathbf{a} \cdot \mathbf{b}$. Two vectors $\mathbf{a}$ and $\mathbf{b}$ are **orthogonal** (perpendicular) to each other if and only if $\mathbf{a} \cdot \mathbf{b} = 0$; see Figure 1.18.

orthogonal

The *Euclidean length*, or L_2**-norm**, of a vector is defined as

$$\|\mathbf{a}\|_2 = (\mathbf{a}^\top \mathbf{a})^{1/2} = \Big(\sum_{j=1}^{p} a_j^2 \Big)^{1/2}.$$

Another common norm is the L_1**-norm**

$$\|\mathbf{a}\|_1 = \sum_{j=1}^{p} |a_j|.$$

Let $\mathbf{A}$ be a $p \times r$ matrix, i.e. and matrix with p rows and r columns:

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1r} \\ a_{21} & a_{22} & \cdots & a_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ a_{p1} & a_{p2} & \cdots & a_{pr} \end{pmatrix}.$$

The **identity matrix** $\mathbf{I}_p$ is the $p \times p$ matrix

identity matrix

$$\mathbf{I}_p = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix},$$

which pays the role of 1 in the world of matrices so that $\mathbf{A}\mathbf{I}_p = \mathbf{I}_p\mathbf{A} = \mathbf{A}$ for any $p \times p$ matrix $\mathbf{A}$.

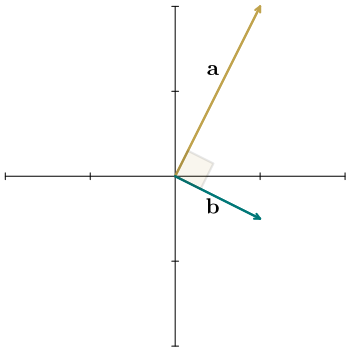

Figure 1.62: Geometric illustration of two orthogonal vectors $\mathbf{a}$ and $\mathbf{b}$.

L_2-norm

L_1-norm

The **matrix-vector product** of an $p \times r$ matrix $\mathbf{A}$ and r-element vector $\mathbf{b} = (b_1, b_2, \ldots, b_r)^\top$ is

matrix-vector product

$$\mathbf{Ab} = \begin{pmatrix} \sum_{j=1}^{r} a_{1j} b_j \\ \sum_{j=1}^{r} a_{2j} b_j \\ \vdots \\ \sum_{j=1}^{r} a_{pj} b_j \end{pmatrix}.$$

Defining $\mathbf{a}_i^\top$ to be the ith row of $\mathbf{A}$ we can write

$$\mathbf{Ab} = \begin{pmatrix} \mathbf{a}_1^\top \mathbf{b} \\ \mathbf{a}_2^\top \mathbf{b} \\ \vdots \\ \mathbf{a}_p^\top \mathbf{b} \end{pmatrix},$$

where $\mathbf{a}_i^\top \mathbf{b} = \sum_{j=1}^{r} a_{ij} b_j$ is a simple vector (dot) product.

Similarly, the **matrix-matrix product** of the $p \times q$ matrix $\mathbf{A}$ and the $q \times r$ matrix $\mathbf{B}$ is defined as

matrix-matrix product

$$\mathbf{AB} = \begin{pmatrix} \mathbf{a}_1^\top \mathbf{b}_1 & \mathbf{a}_1^\top \mathbf{b}_2 & \cdots & \mathbf{a}_1^\top \mathbf{b}_r \\ \mathbf{a}_2^\top \mathbf{b}_1 & \mathbf{a}_2^\top \mathbf{b}_2 & \cdots & \mathbf{a}_2^\top \mathbf{b}_r \\ \vdots & & & \\ \mathbf{a}_p^\top \mathbf{b}_1 & \mathbf{a}_p^\top \mathbf{b}_2 & \cdots & \mathbf{a}_p^\top \mathbf{b}_r \end{pmatrix}.$$

Note the the number of columns in $\mathbf{A}$ must equal the number of rows in $\mathbf{B}$ and the end result of the product is a matrix with dimensions $p \times r$. We use the terminology that $\mathbf{A}$ *pre-multiplies* $\mathbf{B}$ in the product $\mathbf{AB}$, or, equivalently, that $\mathbf{B}$ *post-multiplies* $\mathbf{A}$.

The **matrix transpose** of $p \times r$ matrix $\mathbf{A}$, denoted by $\mathbf{A}^\top$, is the $r \times p$ matrix where the ith column is the i row of $\mathbf{A}$ Let $\mathbf{A}$ be a matrix with p rows and r columns

matrix transpose

$$\mathbf{A}^\top = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{1p} \\ a_{12} & a_{22} & \cdots & a_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1p} & a_{1p} & \cdots & a_{rp} \end{pmatrix}.$$

Determinant and inverse matrix

The **determinant** of a square 2×2 matrix $\mathbf{A}$ is the scalar (i.e. single number)

determinant

$$|\mathbf{A}| = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11} a_{22} - a_{12} a_{21} \tag{1.17}$$

and for a 3×3 matrix

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = \begin{array}{l} a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} \\ -a_{13}a_{22}a_{31} - a_{12}a_{21}a_{33} - a_{11}a_{23}a_{32}, \end{array} \tag{1.18}$$

and increasingly more complex expressions for higher dimensional matrices. The exact expressions are less important here however. It is enough to remember that a determinant of a matrix $\mathbf{A}$ is a scalar that represent the *volume* of the matrix, in the sense that the absolute value of the determinant of $\mathbf{A}$ is the volume of a parallelepiped formed by the columns of $\mathbf{A}$; see Figure 1.18 for an illustration.

We will most often see the determinant of a covariance matrix Σ for a random vector $\mathbf{x}$, where $|\Sigma|$ can then be taken as a measure of *total variance* of $\mathbf{x}$. Let us for concreteness consider the bivariate case with a bivariate normal with mean vector $\boldsymbol{\mu} = (\mu_1, \mu_2)$ and covariance matrix

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}.$$

which has determinant $|\boldsymbol{\Sigma}| = \sigma_1^2\sigma_2^2(1-\rho^2)$. Consider first the case with no correlation, $\rho = 0$, where the total variance is $|\boldsymbol{\Sigma}| = \sigma_1^2\sigma_2^2$. As $\rho \to$ and the variables are increasing correlated and the total variance decreases. When $\rho = 1$ the two variables are perfectly correlated and the total variance is zero. The same is true when $\rho \to -1$ where the variables are perfectly negatively correlated, the total variance becomes smaller and smaller.

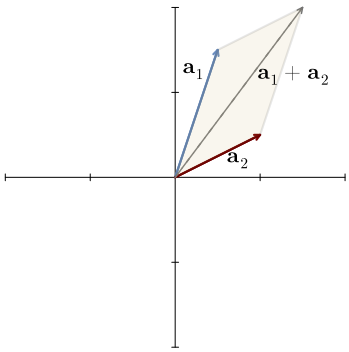

Figure 1.63: Geometric illustration of the determinant as the area of the parallelogram formed by the 2×2 matrix $\mathbf{A} = (\mathbf{a}_1, \mathbf{a}_2)$.

Some rules of determinants are worth noting. First, $|c\mathbf{A}| = c^p|\mathbf{A}|$ for any scalar c and $p \times p$ matrix $\mathbf{A}$. Second, the determinant of a diagonal matrix is just the product of the diagonal elements

$$\begin{vmatrix} a_{11} & 0 & \cdots & 0 \\ 0 & a_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{pp} \end{vmatrix} = a_{11}a_{22}\cdots a_{pp}.$$

The same is true for a lower diagonal matrix, i.e. a matrix where all the elements above the diagonal are zero, but some elements on the diagonal and/or below the diagonal may be non-zero. Finally, for the product of two square matrices $\mathbf{A}$ and $\mathbf{B}$ we have

$$|\mathbf{AB}| = |\mathbf{A}| \cdot |\mathbf{B}|. \tag{1.19}$$

The same type of result holds for a product of three matrices $|\mathbf{ABC}| = |\mathbf{A}| \cdot |\mathbf{B}| \cdot |\mathbf{C}|$ and so on.

The **matrix inverse** of a square $p \times p$ matrix $\mathbf{A}$ is the matrix $\mathbf{A}^{-1}$ matrix inverse

such that

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = I_p. \tag{1.20}$$

Not every square matrix has an inverse, but when it exists it is unique. A sufficient and necessary condition for a square matrix $\mathbf{A}$ to have an inverse is that its column are linearly independent, i.e. that $\sum_{j=1}^{p} \alpha_j \mathbf{a}_j = \mathbf{0}$ only for $\alpha_1 = \alpha_2 = \ldots = \alpha_p = 0$, where $\mathbf{a}_j$ is the jth column of $\mathbf{A}$ and $\mathbf{0}$ is the zero vector. Invertible matrices are also called non-singular. Here are two useful rules for inverses:

$$|\mathbf{A}^{-1}| = \frac{1}{|\mathbf{A}|}$$

and if both $\mathbf{A}$ and $\mathbf{B}$ are invertible then

$$(\mathbf{A}\mathbf{B})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1},$$

where you should note the reverse order of the matrices. The same type of result holds for a product of three matrices $(\mathbf{A}\mathbf{B}\mathbf{C})^{-1} = \mathbf{C}^{-1}\mathbf{B}^{-1}\mathbf{A}^{-1}$.

The **matrix trace** of a matrix $\mathbf{A}$ is simply the sum of its diagonal elements

matrix trace

$$\mathrm{tr}(\mathbf{A}) = \sum_{j=1} a_{jj}. \tag{1.21}$$

The trace has the following circular property

$$\mathrm{tr}(\mathbf{A}\mathbf{B}\mathbf{C}) = \mathrm{tr}(\mathbf{C}\mathbf{A}\mathbf{B}) = \mathrm{tr}(\mathbf{B}\mathbf{C}\mathbf{A}), \tag{1.22}$$

for any square matrices $\mathbf{A}$,$\mathbf{B}$ and $\mathbf{C}$ with the same dimensions.

*Partitioned matrices**

Consider a *partitioned matrix* of dimensions $p \times p$

$$\mathbf{A} = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix}, \tag{1.23}$$

where $\mathbf{A}_{11}$ is of dimensions $p_1 \times p_1$, $\mathbf{A}_{22}$ is of dimensions $p_2 \times p_2$, $\mathbf{A}_{12}$ and $\mathbf{A}_{21}$ are of dimensions $p_1 \times p_2$ and $p_2 \times p_1$ respectively. Hence, $p = p_1 + p_2$. The determinant can be then be expressed

$$|\mathbf{A}| = |\mathbf{A}_{11}||\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12}| = |\mathbf{A}_{22}||\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21}|.$$

and the inverse

$$\mathbf{A}^{-1} = \begin{pmatrix} \mathbf{A}^{(11)} & -\mathbf{A}^{(11)}\mathbf{A}_{12}\mathbf{A}_{22}^{-1} \\ -\mathbf{A}_{22}^{-1}\mathbf{A}_{21}\mathbf{A}^{(11)} & \left(\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12}\right)^{-1} \end{pmatrix},$$

where $\mathbf{A}^{(11)} = \left(\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21}\right)^{-1}$.

*Linear transformation, eigendecomposition and principal components**

Consider a linear transformation $\mathbf{y} = \mathbf{m} + \mathbf{A}\mathbf{x}$ from $\mathbf{x}$ to $\mathbf{y}$, where $\mathbf{y}$ and $\mathbf{m}$ are p-dimensional vectors, $\mathbf{x}$ is an q-dimensional vector, and $\mathbf{A}$ is a $p \times q$ matrix. If $\mathbf{x}$ is a random vector with mean $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$ then

$$\mathbb{E}(\mathbf{y}) = \mathbf{m} + \mathbf{A}\boldsymbol{\mu} \tag{1.24}$$

$$\mathbb{V}(\mathbf{y}) = \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^\top \tag{1.25}$$

Let $p = 1$ so that $\mathbf{A} = \mathbf{a}^\top$ is a r-dimensional row vector. Then $y = m + \mathbf{a}^\top\mathbf{x} = m + \sum_{i=1}^r a_i x_i$ is a scalar, and $\mathbb{V}(y) = \mathbf{a}^\top\boldsymbol{\Sigma}\mathbf{a}$. Since we require a variance to be positive we must require that the covariance matrix $\boldsymbol{\Sigma}$ satisfies $\mathbf{a}^\top\boldsymbol{\Sigma}\mathbf{a} > 0$ for all $\mathbf{a} \neq \mathbf{0}$. We say that $\boldsymbol{\Sigma}$ must be **positive definite**. A matrix $\boldsymbol{\Sigma}$ is positive definite if and only if $|\boldsymbol{\Sigma}| > 0$. If we allow that the variance can also be exactly zero, then we require $\boldsymbol{\Sigma}$ to be positive semidefinite, sometimes abbreviated by psd or p.s.d.

positive definite

An **eigenvector** $\mathbf{v}$ of an invertible matrix $\mathbf{A}$ is a vector that keeps its direction when transformed by $\mathbf{A}$, i.e.

eigenvector

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v},$$

where λ is the **eigenvalue** associated with the eigenvector $\mathbf{v}$. Note how the transformation only leads to a scaling of $\mathbf{v}$ by λ, but the direction of the vector remains the same. A non-singular $p \times p$ matrix $\mathbf{A}$ has p linearly independent eigenvectors, $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_p$ each associated with its own eigenvalue $\lambda_1, \lambda_2, \ldots, \lambda_p$. Eigenvectors are normalized to have unit length, i.e. $\mathbf{v}_j^\top\mathbf{v}_j = 1$ for $j = 1, \ldots, p$ and to be orthogonal to each other, i.e. $\mathbf{v}_i^\top\mathbf{v}_j = 0$ for $i \neq j$. We can therefore collect all eigenvectors into a $p \times p$ *orthonormal* matrix $\mathbf{V} = (\mathbf{v}_1, \ldots, \mathbf{v}_p)$ with the property $\mathbf{V}^\top\mathbf{V} = \mathbf{V}\mathbf{V}^\top = \mathbf{I}_p$; note that the inverse of an orthonormal matrix is simply its transpose. We can now write

eigenvalue

$$\mathbf{A}\mathbf{V} = \mathbf{V}\boldsymbol{\Lambda}, \tag{1.26}$$

where $\boldsymbol{\Lambda} = \text{Diag}(\lambda_1, \ldots, \lambda_p)$ is a diagonal matrix of eigenvalues. We therefore obtain the **spectral decomposition** of the invertible matrix $\mathbf{A}$ by post-multiplying both sides of (1.26) with $\mathbf{V}^\top$ (since $\mathbf{V}\mathbf{V}^\top = \mathbf{I}_p$)

spectral decomposition

$$\mathbf{A} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^\top. \tag{1.27}$$

The spectral decomposition gives us a connection between the determinant and inverse of a matrix and its eigenvalues and eigenvectors. The determinant can be written

$$|\mathbf{A}| = |\mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^\top| = |\mathbf{V}||\boldsymbol{\Lambda}||\mathbf{V}^\top| = |\boldsymbol{\Lambda}||\mathbf{V}\mathbf{V}^\top| = \prod_{j=1}^p \lambda_j,$$

since the determinant of a diagonal matrix is the product of its diagonal elements and $\mathbf{V}\mathbf{V}^\top = \mathbf{I}_p$ so $|\mathbf{V}\mathbf{V}^\top| = 1$. Given that a matrix is positive definite if its determinant is non-zero, this shows that a matrix is positive definite if and only if all of its eigenvalues are positive.

Recall that the inverse of an orthonormal matrix is its transpose $\mathbf{V}^{-1} = \mathbf{V}^\top$. We can use the product rule for inverses to express the inverse of $\mathbf{A}$ as

$$\mathbf{A}^{-1} = (\mathbf{V}^\top)^{-1}\mathbf{\Lambda}^{-1}\mathbf{V}^{-1} = \mathbf{V}\mathbf{\Lambda}^{-1}\mathbf{V}^\top,$$

and $\mathbf{\Lambda}^{-1} = \text{Diag}(1/\lambda_1, \ldots, 1/\lambda_p)$. There are more general decompositions of matrices, also for non-square and non-invertible matrices, the most famous being the singular value decomposition (Harville, 1998).

Finally, using the circular property of the trace in (1.22), we see that the trace of matrix is the sum of its eigenvalues

$$\text{tr}(\mathbf{A}) = \text{tr}(\mathbf{V}\mathbf{\Lambda}\mathbf{V}^\top) = \text{tr}(\mathbf{V}^\top\mathbf{V}\mathbf{\Lambda}) = \text{tr}(\mathbf{I}_p\mathbf{\Lambda}) = \text{tr}(\mathbf{\Lambda}) = \sum_{j=1}^{p} \lambda_j.$$

Consider now the spectral value decomposition $\mathbf{\Sigma} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^\top$ on a covariance matrix $\mathbf{\Sigma}$ of a random vector $\mathbf{x}$. The linear transformation $\mathbf{y} = \mathbf{V}^\top\mathbf{x}$ has an interesting covariance matrix

$$\mathbb{V}(\mathbf{y}) = \mathbf{V}^\top\mathbf{\Sigma}\mathbf{V} = \mathbf{V}^\top(\mathbf{V}\mathbf{\Lambda}\mathbf{V}^\top)\mathbf{V} = \mathbf{\Lambda}. \tag{1.28}$$

Hence, the new variables in $y_j = \mathbf{v}_j^\top\mathbf{x}$ for $j = 1, \ldots, p$ are uncorrelated and have the eigenvalues as variances: $\mathbb{V}(y_j) = \lambda_j$. These variables are called the **principal components** of $\mathbf{x}$. If we order the eigenvalues in descending order $\lambda_1 \geq \cdots \geq \lambda_p$ then the first principal component $y_1 = \mathbf{v}_1^\top\mathbf{x}$ is the linear combination of the variables in $\mathbf{x}$ with maximal variance, the second principal component $y_2 = \mathbf{v}_2^\top\mathbf{x}$ is the linear combination with maximal variance subject to being uncorrelated with y_1 and so on. Summarizing a possibly high-dimensional correlated $\mathbf{x}$ with the $r < p$ largest principal components is therefore a useful way to compress the data while retaining most of the variance. Figure 1.64 illustrates the transformation of sampled data into uncorrelated principal components.

principal components

*Matrix powers and the Cholesky decomposition**

The spectral decomposition is useful for defining powers of a matrix. Let $\mathbf{A}$ be a square non-singular matrix with spectral decomposition $\mathbf{V}\mathbf{\Lambda}\mathbf{V}^\top$. Then since $\mathbf{V}$ is orthonormal we have

$$\mathbf{A}^2 = \mathbf{A}\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^\top\mathbf{V}\mathbf{\Lambda}\mathbf{V}^\top = \mathbf{V}\mathbf{\Lambda}^2\mathbf{V}^\top,$$

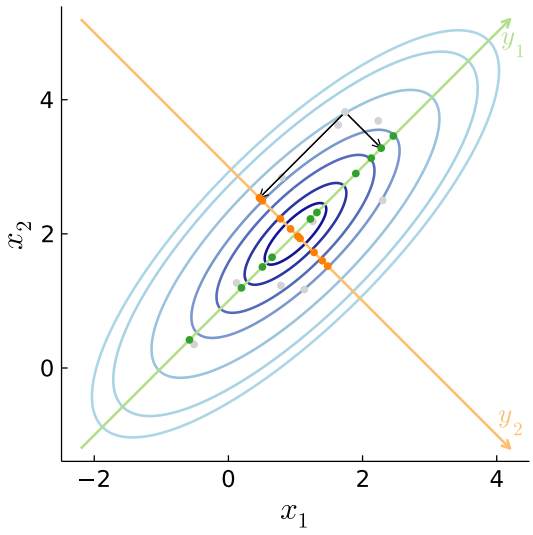

Figure 1.64: Illustration of principal components from data points sampled from a multivariate normal distribution with mean $\boldsymbol{\mu} = (1,2)^\top$ and correlation $\rho = 0.8$. The sampled data points are shown in light gray and their projections onto the first principal components axis (y_1) are shown as green points and as orange points when projected against the second principal component axis (y_2); this projection is illustrated by arrows for one of the data points. The larger variability of the green points along the y_1 axis compared to the variability of the orange points along the y_2 is reflected in the eigenvalues $\lambda_1 = 1.8 > \lambda_2 = 0.2$.

where $\boldsymbol{\Lambda}^2 = \text{Diag}(\lambda_1^2, \ldots, \lambda_p^2)$. Continuing by multiplying with additional $\mathbf{A}$ factors we have for any positive integer k the **matrix power**

matrix power

$$\mathbf{A}^k = \mathbf{V}\boldsymbol{\Lambda}^k\mathbf{V}^\top.$$

We can extend this to any power k, not necessarily a positive integer, and in particular to $k = 1/2$ to define a **matrix square root** $\mathbf{A}^{1/2} = \mathbf{V}\boldsymbol{\Lambda}^{1/2}\mathbf{V}^\top$ with the property $\mathbf{A}^{1/2}\mathbf{A}^{1/2} = \mathbf{A}$. This construction can be used to simulate $\mathbf{x} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ by

matrix square root

$$\mathbf{x} = \boldsymbol{\mu} + \boldsymbol{\Sigma}^{1/2}\mathbf{z}, \tag{1.29}$$

where $\mathbf{z}$ is a p-dimensional vector with independent standard normal variables. Since linear transformations of normal variables are normal, $\mathbf{x}$ is multivariate normal with mean $\boldsymbol{\mu}$ and covariance matrix $\mathbb{V}(\mathbf{x}) = \boldsymbol{\Sigma}^{1/2}\mathbb{V}(\mathbf{z})\boldsymbol{\Sigma}^{1/2} = \boldsymbol{\Sigma}^{1/2}\mathbf{I}_p\boldsymbol{\Sigma}^{1/2} = \boldsymbol{\Sigma}$ as required. The spectral decomposition is just one way of defining a matrix square root. Another commonly used matrix square root is the **Cholesky decomposition**

Cholesky decomposition

$$\mathbf{A} = \mathbf{L}\mathbf{L}^\top, \tag{1.30}$$

where

$$\mathbf{L} = \begin{pmatrix} l_{11} & 0 & 0 & \cdots & 0 \\ l_{21} & l_{22} & 0 & \cdots & 0 \\ l_{31} & l_{32} & l_{33} & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & 0 \\ l_{p1} & l_{p2} & \ldots & l_{p,p-1} & l_{pp} \end{pmatrix}$$

is a lower triangular matrix. The Cholesky square root can equally well be used for multivariate normal simulation: if $\mathbf{\Sigma} = \mathbf{L}\mathbf{L}^\top$ then $\mathbf{x} = \boldsymbol{\mu} + \mathbf{L}\mathbf{z} \sim N(\boldsymbol{\mu}, \mathbf{\Sigma})$, where again $\mathbf{z}$ is a p-dimensional vector with independent standard normal variables. The Cholesky decomposition makes it possible to compute the multivariate normal density cheaply since

$$\begin{aligned} p(\mathbf{x}) &= |2\pi\mathbf{\Sigma}|^{-1/2} \exp\Big(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top \mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\Big) \\ &= (2\pi)^{-p/2}|\mathbf{L}\mathbf{L}^\top|^{-1/2} \exp\Big(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top (\mathbf{L}\mathbf{L}^\top)^{-1}(\mathbf{x}-\boldsymbol{\mu})\Big) \\ &= (2\pi)^{-p/2}|\mathbf{L}|^{-1} \exp\Big(-\frac{1}{2}\mathbf{y}^\top\mathbf{y}\Big), \end{aligned} \tag{1.31}$$

where $\mathbf{y} = \mathbf{L}^{-1}(\mathbf{x}-\boldsymbol{\mu})$ and $|\mathbf{L}| = \prod_{j=1}^{p} l_{jj}$ since $\mathbf{L}$ is lower triangular. We can compute $\mathbf{y} = \mathbf{L}^{-1}(\mathbf{x}-\boldsymbol{\mu})$ without explicitly inverting $\mathbf{L}$ by solving the system of equations $\mathbf{L}\mathbf{y} = \mathbf{x}-\boldsymbol{\mu}$ for $\mathbf{y}$. Since $\mathbf{L}$ is lower triangular this can be solved quickly using forward/backward substitution. Note that we have used several of the above mentioned results for determinants and inverses in (1.31), so verifying this derivation is a useful exercise.

*Vector differentiation**

Let $f(\mathbf{x})$ be a scalar valued function of an p-dimensional vector $\mathbf{x}$. The gradient of $f(\mathbf{x})$ with respect to $\mathbf{x}$ is the p-dimensional vector with partial derivatives

$$\frac{\partial}{\partial \mathbf{x}} f(\mathbf{x}) = \begin{pmatrix} \frac{\partial}{\partial x_1} f(\mathbf{x}) \\ \vdots \\ \frac{\partial}{\partial x_p} f(\mathbf{x}) \end{pmatrix}$$

The gradient is sometimes written $\nabla_{\mathbf{x}} f(\mathbf{x})$. For a linear function $f(\mathbf{x}) = \mathbf{a}^\top\mathbf{x}$ for some p-dimensional vector $\mathbf{a}$ the gradient is easily seen to be

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{a}^\top\mathbf{x} = \mathbf{a},$$

matching up with the one-dimensional case $\frac{d}{dx}ax = a$. For a quadratic function $f(\mathbf{x}) = \mathbf{x}^\top\mathbf{A}\mathbf{x}$ for some square matrix $\mathbf{A}$, often called a quadratic form, we have the gradient

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{x}^\top\mathbf{A}\mathbf{x} = 2\mathbf{A}\mathbf{x},$$

which also matches the one-dimensional case $\frac{d}{dx}ax^2 = 2ax$.

Consider now a *multi-output* function $\mathbf{y} = \mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), \ldots, f_p(\mathbf{x}))^\top$ with p-dimensional output $\mathbf{y}$ and q-dimensional input $\mathbf{x}$. The $p \times q$

matrix of partial derivatives

$$\frac{\partial}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}) = \begin{pmatrix} \frac{\partial}{\partial x_1} f_1(\mathbf{x}) & \frac{\partial}{\partial x_2} f_1(\mathbf{x}) & \cdots & \frac{\partial}{\partial x_q} f_1(\mathbf{x}) \\ \vdots & & & \\ \frac{\partial}{\partial x_1} f_p(\mathbf{x}) & \frac{\partial}{\partial x_2} f_p(\mathbf{x}) & \cdots & \frac{\partial}{\partial x_q} f_p(\mathbf{x}) \end{pmatrix}.$$

is called the **Jacobian matrix**. For a linear multi-output function $\mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x}$ we have $\frac{\partial}{\partial \mathbf{x}}\mathbf{A}\mathbf{x} = \mathbf{A}$.

Jacobian matrix

Recall that the **chain rule** for differentiation of the function composition $f(x) = g(h(x))$ is the product of the so called outer and inner derivatives: $\frac{d}{dx}f(x) = \frac{d}{dz}g(z)\frac{d}{dx}h(x)$. The chain rule for a multivariable function composition $f(\mathbf{x}) = g(h(\mathbf{x}))$, where $h : \mathbb{R}^p \to \mathbb{R}^q$ and $g : \mathbb{R}^q \to \mathbb{R}$, is similar

chain rule

$$\frac{\partial}{\partial \mathbf{x}} f(\mathbf{x}) = \left(\frac{\partial}{\partial \mathbf{x}} h(\mathbf{x})\right)^\top \frac{\partial}{\partial \mathbf{z}} g(\mathbf{z}),$$

where $\mathbf{z} = h(\mathbf{x})$ is in general a mapping $\mathbf{x} \to \mathbf{z}$ from $\mathbb{R}^p$ to $\mathbb{R}^q$, so that $\frac{\partial}{\partial \mathbf{x}} h(\mathbf{x})$ is a $q \times p$ Jacobian matrix when both $p > 1$ and $q > 1$.

As an example on how to use the above rules for differentiation, consider deriving the least squares estimator in linear regression obtained by minimizing the residual sum of squares

$$Q(\boldsymbol{\beta}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) = \mathbf{e}(\boldsymbol{\beta})^\top \mathbf{e}(\boldsymbol{\beta}),$$

where $\mathbf{e}(\boldsymbol{\beta}) = \mathbf{y} - \mathbf{X}\boldsymbol{\beta}$ is the vector of residuals. The least squares estimate is therefore the solution to $\frac{\partial}{\partial \boldsymbol{\beta}} Q(\boldsymbol{\beta}) = \mathbf{0}$ where

$$\frac{\partial}{\partial \boldsymbol{\beta}} Q(\boldsymbol{\beta}) = \left(\frac{\partial}{\partial \boldsymbol{\beta}} \mathbf{e}(\boldsymbol{\beta})\right)^\top \frac{\partial}{\partial \mathbf{e}} \mathbf{e}^\top \mathbf{e} = \left(\frac{\partial}{\partial \boldsymbol{\beta}} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})\right)^\top 2\mathbf{e} = -2\mathbf{X}^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}).$$

Hence the least squares estimator is the solution to $\mathbf{X}^\top \mathbf{y} = \mathbf{X}^\top \mathbf{X}\boldsymbol{\beta}$. If the columns of $\mathbf{X}$ are linearly independent then the inverse $\left(\mathbf{X}^\top \mathbf{X}\right)^{-1}$ exist and we can multiply both sides with it to get the least squares solution $\hat{\boldsymbol{\beta}} = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{y}$.

EXERCISES

Linear algebra

1. Some linear algebra problem here.

2 Probability

2.1 Probabilities of events

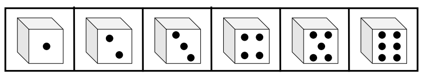

Figure 2.1: The outcome space for a single die throw.

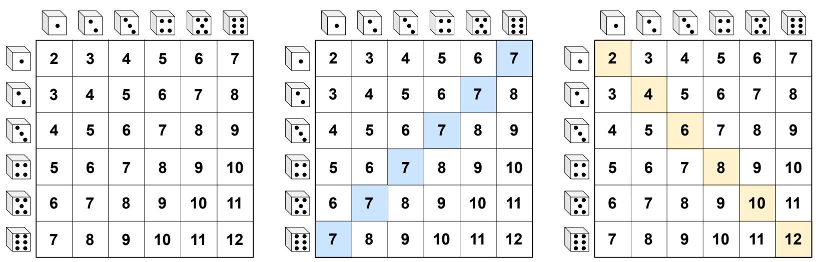

Figure 2.2: Throw of two dice.
Left: the outcome space.
Middle: the event 'sum of seven'

$A = \{(1,6), (2,5), (3,4), (4,3), (5,2), (6,1)\}$

Right: the event 'same on both dice'

$B = \{(1,1), (2,2), (3,3), (4,4), (5,5), (6,6)\}$

2.2 Conditional Probabilities for events

2.3 Random variables and Probability distributions

interest rate in %	probability	monthly cost
1	0.017	833
2	0.094	1667
3	0.252	2500
4	0.334	3333
5	0.219	4167
6	0.071	5000
7	0.011	5833
8	0.001	6667

Basic rules for probabilities of events

Let A and B be two events in a sample space S.

Universal and empty set

$\Pr(S) = 1$ and $\Pr(\emptyset) = 0$

Complement rule

$\Pr(A) = 1 - \Pr(A^c)$

Addition rule

$\Pr(A \cup B) = \Pr(A) + \Pr(B) - \Pr(A \cap B)$

$\Pr(A \cup B) = \Pr(A) + \Pr(B)$ when A and B are disjoint

Multiplication rule

$\Pr(A \cap B) = \Pr(A|B)\Pr(B)$

$\Pr(A \cap B) = \Pr(A)\Pr(B)$ when A and B are independent

Figure 2.3: Basic rules for probabilities of events.

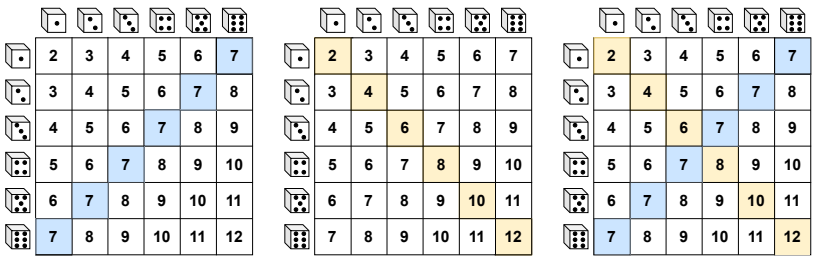

Figure 2.4: Throw of two dice.
Left: the event 'sum of seven'

$A = \{(1,6),(2,5),(3,4),(4,3),(5,2),(6,1)\}$

Middle: the event 'same on both dice'

$B = \{(1,1),(2,2),(3,3),(4,4),(5,5),(6,6)\}$

Right: The intersection of these two event $A \cap B = \emptyset$ is the empty event.

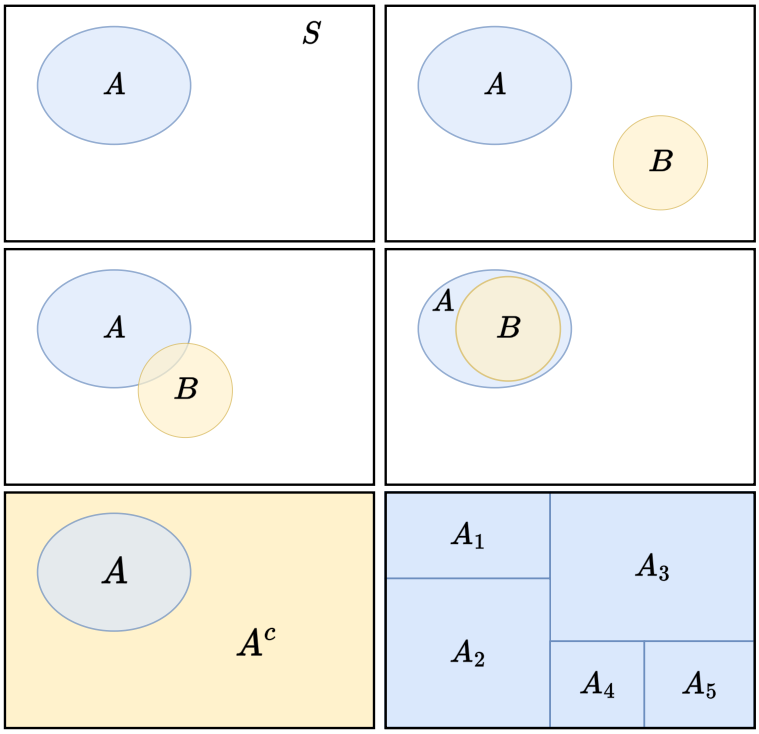

Figure 2.5: Events in a sample space S.
Top left: event A.
Top right: two disjoint events A and B with no common elements.
Middle left: two events A and B with some common elements.
Middle right: A is a subset of event B.
Bottom left: A^c is the complement of event A.
Bottom right: $A_1, \ldots, A_5$ is a partition of the sample space.

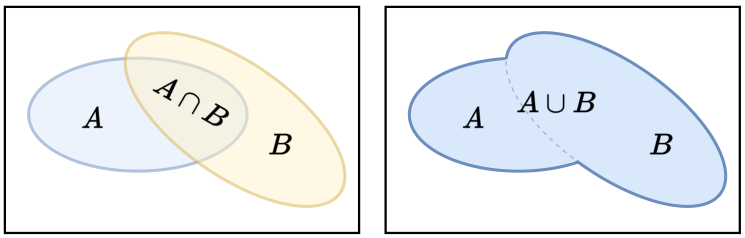

Figure 2.6: Intersection and union.

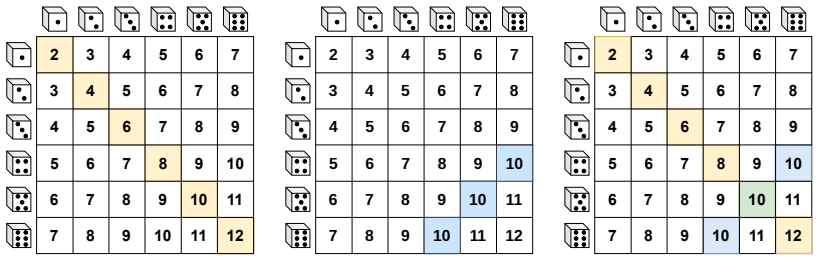

Figure 2.7: Right: the event 'same on both dice' $B = \{(1,1),(2,2),(3,3),(4,4),(5,5),(6,6)\}$ marked out in yellow. Middle: the event 'sum is ten' $C = \{(4,6),(5,5),(6,4)\}$ marked out in blue. Right: The intersection of these two event $B \cap C = \{(5,5)\}$ is marked out in green.

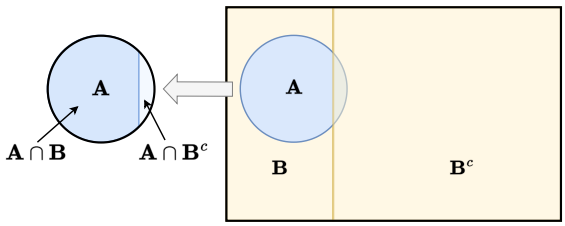

Figure 2.8: Illustrating how conditioning on the event A makes A the new sample space. The conditional probability of another event B is calculated as the ratio of the intersection between A and B to the area of the new sample space A.

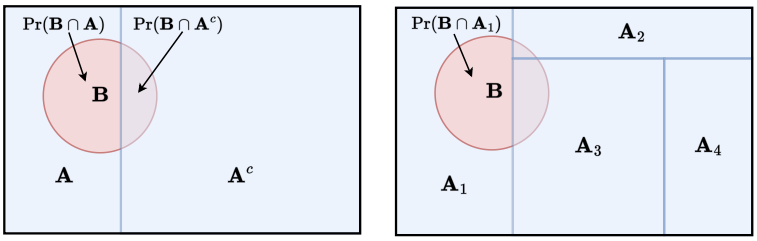

Figure 2.9: Law of total probability.

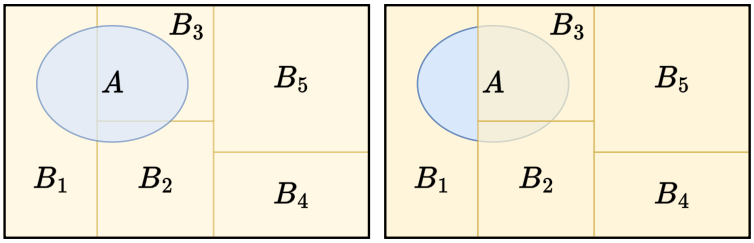

Figure 2.10: Bayes theorem for events.

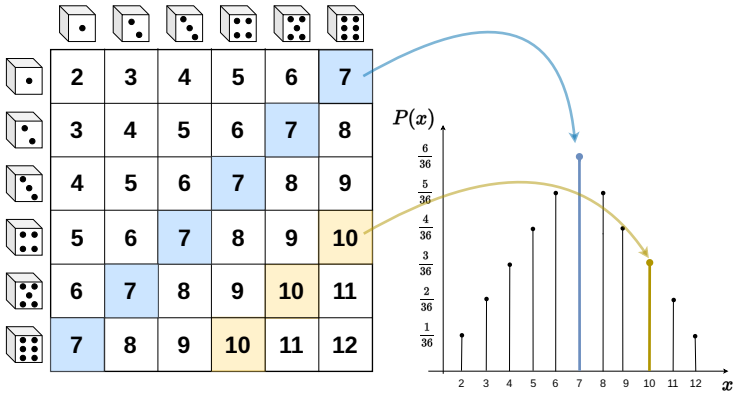

Figure 2.11: Illustrating the how the outcome from throwing two dice implies a probability distribution for the random variable $X =$ sum of the two dice. The probability distribution is given by the height of the bars.

Expected value

Definition. *The **expected value** or **mean** of a discrete random variable X with support $\mathcal{X} = \{x_1, x_2, \ldots, x_K\}$ is defined as*

$$\mu = \mathbb{E}(X) = \sum_{k=1}^{K} x_k \cdot P(X = x_k)$$

Definition. *The **expected value** or **mean** of a continuous random variable X with support $\mathcal{X}$ and probability density $p(x)$ is defined as*

$$\mu = \mathbb{E}(X) := \int_{\mathcal{X}} x \cdot p(x)\, \mathrm{d}x$$

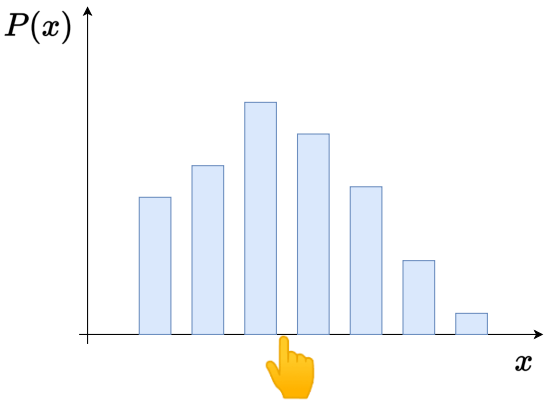

Figure 2.12: Mean as the balance point of a distribution. The mean is the point where the distribution would balance if it was a physical object.

EXAMPLE: Interest rate on a loan.

$$\mathbb{E}(\text{cost}) = 417 \cdot 0.017 + 833 \cdot 0.094 + \ldots 3333 \cdot 0.001 \approx 1626 \text{ EUR}$$

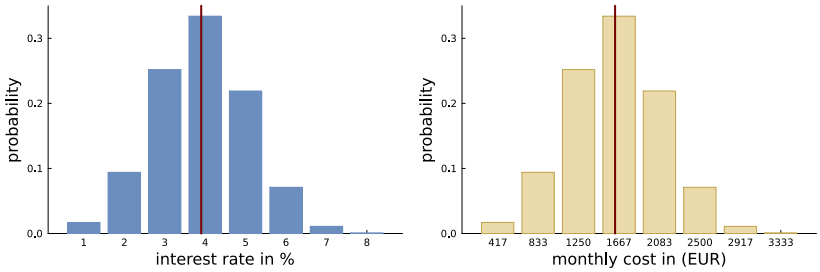

Figure 2.13: The probability distribution for next year's interest rate on a loan (left) and the corresponding monthly cost (right). The mean in each distribution is marked with a vertical red line.

Variance

Definition. *The **variance** of a discrete random variable X with support $\mathcal{X} = \{x_1, x_2, \ldots, x_K\}$ and mean μ is defined as*

$$\mathbb{V}(X) := \sum_{k=1}^{K} (x_k - \mu)^2 \cdot P(X = x_k)$$

Definition. *The **variance** of a continuous random variable X with support $\mathcal{X}$, mean μ and probability density $p(x)$ is defined as*

$$\mathbb{V}(X) := \int_{\mathcal{X}} (x - \mu)^2 \cdot p(x)\, \mathrm{d}x$$

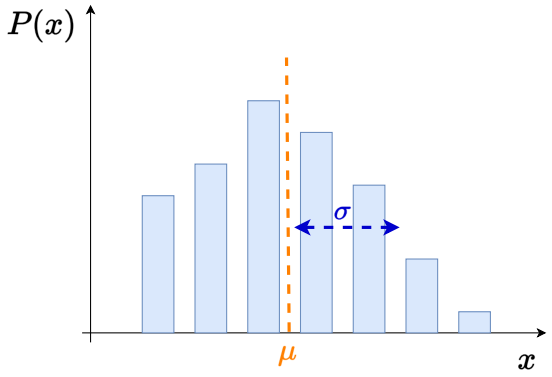

Figure 2.14: Variance measures the spread of the distribution as the (squared) average distance to the mean.

EXAMPLE: Interest rate on a loan.

$$\begin{aligned}\mathbb{V}(\text{cost}) =& (417 - 3252)^2 \cdot 0.017 + (833 - 1626)^2 \cdot 0.094 + \ldots \\ &+ (3333 - 1626)^2 \cdot 0.001 \approx 241368 \text{ EUR}^2\end{aligned}$$

and the standard deviation is $\sigma = \sqrt{\mathbb{V}(\text{cost})} \approx 491$ EUR.

2.4 *Mean and variance of linear combinations of random variables*

Mean and variance of a linear transformation

Shift with constant c

$\mathbb{E}(X + c) = \mathbb{E}(X) + c$ $\quad$ $\mathbb{V}(X + c) = \mathbb{V}(X)$

Scaling with constant a

$\mathbb{E}(a \cdot X) = a \cdot \mathbb{E}(X)$ $\quad$ $\mathbb{V}(a \cdot X) = a^2\mathbb{V}(X)$

Linear transformation

$\mathbb{E}(c + a \cdot X) = c + a \cdot \mathbb{E}(X)$ $\quad$ $\mathbb{V}(c + a \cdot X) = a^2\mathbb{V}(X)$

Figure 2.15: Mean and variance for a shift, scaling and linear transformation of a random variable.

Mean and variance of a sum of independent variables

If X and Y are independent random variables, then

Sum of two random variables

$\mathbb{E}(X + Y) = \mathbb{E}(X) + \mathbb{E}(Y)$

$\mathbb{V}(X + Y) = \mathbb{V}(X) + \mathbb{V}(X)$

Linear transformation

$\mathbb{E}(a \cdot X + b \cdot Y) = a \cdot \mathbb{E}(X) + b \cdot \mathbb{E}(Y)$

$\mathbb{V}(a \cdot X + b \cdot Y) = a^2\mathbb{V}(X) + b^2\mathbb{V}(Y)$

If $X_1, \ldots, X_n$ are independent random variables, then

Sum of n random variables

$\mathbb{E}(X_1 + \ldots + X_n) = \mathbb{E}(X_1) + \ldots + \mathbb{E}(X_n)$

$\mathbb{V}(X_1 + \ldots + X_n) = \mathbb{V}(X_1) + \ldots + \mathbb{V}(X_n)$

Figure 2.16: Mean and variance for a shift, scaling and linear transformation of a random variable.

3 Discrete random variables

3.1 Bernoulli distribution

Definition. *A* Bernoulli(p) *trial is an experiment that*

- *has only two possible outcomes, success and failure.*
- *the success probability is* p

Bernoulli distribution

$$X \sim \text{Bern}(p), \text{ with support } X \in \{0, 1\}$$

Probability function

$$p(x) = \begin{cases} q & \text{for } x = 0 \\ p & \text{for } x = 1 \end{cases} \tag{3.1}$$

Expected value

$$\mathbb{E}(X) = p$$

Variance

$$\mathbb{V}(X) = pq$$

Figure 3.1: Properties of the Bernoulli distribution.

3.2 *Binomial distribution*

Definition. *A **binomial random variable***

$$X \sim \text{Binom}(n, p), \text{ with support } X \in \{0, 1, 2, \ldots, n\}$$

*counts the number of **successes** in n independent* Bernoulli(p) *trials.*

Binomial distribution

$$X \sim \text{Binom}(n, p), \text{ with support } X \in \{0, 1, 2, \ldots, n\}$$

Probability function

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

Expected value

$$\mathbb{E}(X) = np$$

Variance

$$\mathbb{V}(X) = npq$$

Figure 3.2: Properties of the binomial distribution.

Here we need to count how many ways we can obtain x successes and $n - x$ failures in a total of n trials. For example, in an experiment with $n = 4$ trials, where we observe exactly $x = 2$ successes, the number of ways that this can happen is given by $\binom{4}{2} = \frac{4!}{2!2!} = \frac{4 \cdot 3 \cdot 2 \cdot 1}{2 \cdot 1 \cdot 2 \cdot 1} = \frac{24}{4} = 6$. Figure 3.3 lists all possible combinations one can obtain x successes (1) and $n - x$ failures (0) in $n = 4$ trials.

To see the connection with the selection of colored balls Section 1.5, we can let each of the four trials corresponds to a coloured ball, which for clarity can also have different numbers from 1 to 4; see Figure 3.5. Drawing a ball with the number i means that a success occurred on trial i. Since we are interested in the number of ways that we can distribute $k = 2$ successes over $n = 4$ trials, this corresponds to drawing $k = 2$ balls without replacement and without regard to order. Each outcome in the table in Figure 3.4 also lists the corresponding selection of colored balls. For example, the outcome 1, 0, 1, 0, i.e. the two successes occurred on the first and third trials, corresponds to drawing the ball with number 1 on the first draw, and the ball with number 3 on the second draw, *or* drawing the ball with number 3 on the first draw, and the ball with number 1 on the second

$\binom{4}{0} = 1$

x_1	x_2	x_3	x_4	$\sum x_i$
0	0	0	0	0

$\binom{4}{1} = 4$

x_1	x_2	x_3	x_4	$\sum x_i$
1	0	0	0	1
0	1	0	0	1
0	0	1	0	1
0	0	0	1	1

$\binom{4}{2} = 6$

x_1	x_2	x_3	x_4	$\sum x_i$
1	1	0	0	2
1	0	1	0	2
1	0	0	1	2
0	1	1	0	2
0	1	0	1	2
0	0	1	1	2

$\binom{4}{4} = 4$

x_1	x_2	x_3	x_4	$\sum x_i$
1	1	1	0	3
1	1	0	1	3
1	0	1	1	3
0	1	1	1	3

Figure 3.3: Listing the number of ways one can obtain x successes (1) and $n - x$ failures (0) in $n = 4$ trials.

Trial 1	Trial 2	Trial 3	Trial 4
1	1	0	0
1	0	1	0
1	0	0	1
0	1	1	0
0	1	0	1
0	0	1	1

Figure 3.4: Listing the number of ways one can obtain two successes (S) and two failures (F) in $n = 4$ trials.

draw.

Figure 3.5: Four colored balls with numbers from 1 to 4.

3.3 *Geometric distribution*

Definition. *A **geometric random variable***

$$X \sim \text{Geom}(p), \text{ with support } X \in \{0, 1, 2, \ldots\}$$

*counts the number of **failures** before the first success in a sequence of independent* Bernoulli(p) *trials.*

geometric distribution

$$X \sim \text{Geom}(p), \text{ with support } X \in \{0, 1, 2, \ldots\}$$

Probability function

$$p(x) = q^x p$$

Expected value

$$\mathbb{E}(X) = \frac{1-p}{p}$$

Variance

$$\mathbb{V}(X) = \frac{1-p}{p^2}$$

Figure 3.6: Properties of the geometric distribution.

3.4 *Poisson distribution*

3.5 *Negative binomial distribution*

Definition. *A **negative binomial random variable***

$$X \sim \text{NegBinom}(r, p), \text{ with support } X \in \{0, 1, 2, \ldots\}$$

*counts the number of **failures** before the rth success in a sequence of independent* Bernoulli(p) *trials.*

An alternative parameterization of the negative binomial distribution has the mean μ as an explicit parameter obtained from the

Poisson distribution

$$X \sim \text{Poisson}(\mu), \text{ with support } X \in \{0, 1, 2, \ldots\}$$

Probability function

$$p(x) = \frac{\mu^x e^{-\mu}}{x!}$$

Expected value

$$\mathbb{E}(X) = \mu$$

Variance

$$\mathbb{V}(X) = \mu$$

Figure 3.7: Properties of the Poisson distribution.

Negative binomial distribution

$$X \sim \text{NegBinom}(r, p), \text{ with support } X \in \{0, 1, 2, \ldots\}$$

Probability function

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

Expected value

$$\mathbb{E}(X) = \frac{r(1-p)}{p}$$

Variance

$$\mathbb{V}(X) = \frac{r(1-p)}{p^2}$$

Figure 3.8: Properties of the negative binomial distribution.

x_1	x_2	x_3	x_4
1	0	0	1
0	1	0	1
0	0	1	1

$$\binom{n-1}{r-1} = \binom{3}{1} = 3$$

Figure 3.9: Enumerating all $\binom{3}{1} = 3$ outcomes where it took $x = 4$ trials before getting a pre-determined number of $r = 2$ successes.

original negative binomial distribution with $p = \frac{r}{r+\mu}$. It is easy to see that with this choice we have $\mathbb{E}(X) = \mu$.

Negative binomial distribution - mean parameterization

$$X \sim \text{NegBinom}(r, \mu), \text{ with support } X \in \{0, 1, 2, \ldots\}$$

Probability function

$$p(x) = \binom{x+r-1}{x} \left(\frac{r}{r+\mu}\right)^r \left(\frac{\mu}{r+\mu}\right)^{x-r}$$

Expected value

$$\mathbb{E}(X) = \mu$$

Variance

$$\mathbb{V}(X) = \mu\left(1 + \frac{\mu}{r}\right)$$

Figure 3.10: Properties of the negative binomial distribution in the mean parameterization.

Recall that the Poisson distribution had the implicit restriction with equal mean and variance, which called **equi-dispersed**. The negative binomial is instead **over-dispersed**: its variance is larger than the mean. When $r \to \infty$ the NegBinom(r, μ) distribution converges to the Poisson(μ) distribution. An estimate of the parameter r in the negative binomial that is very large is therefore an indication that the simpler Poisson distribution might be sufficient to model the data. Conversely, a small estimate of r is a clear signal that the data is over-dispersed and the more general over-dispersed negative binomial distribution is a better model than the equi-dispersed Poisson model. In the more unusual case with *under-dispersed* data, neither of these two models are adequate.

equi-dispersed

over-dispersed

3.6 *Multinomial distribution*

4 Continuous random variables

A *discrete* random variable can take a finite number of outcomes, e.g. $X \in \{x_1, \ldots, x_n\}$, or a countable number of outcomes $X \in \{0, 1, 2, \}$. The values do not need to be integers, but there must be a finite or countable number of different values. A *continuous random variable* has outcomes that can be *any* real value in a given interval. For example, the time delay in the arrival of a bus to a bus stop is a continuous random variable. It can take any value in the interval $[0, \infty)$ down to milliseconds, nanoseconds or whatever precision we can use to measure the time in. A continuous random variable can therefore have potentially infinite number of decimal digits.

The fact that a random variable can take any value makes it impossible to assign a probability to any specific value. One way to think about this is that a continuous random variable has infinite number of digits, and observing a number with exactly the same digits has probability zero. What we can do instead is to assign probabilities to intervals. For example, that the bus delay is at most five minutes or that the delay is between 5 and 10 minutes.

4.1 The cumulative distribution function and the probability density function

The **cumulative distribution function** (**cdf**) of a random variable is defined is defined as

cumulative distribution function

cdf

> **Definition.** *The cumulative distribution function (cdf) of a random variable is defined as*
>
> $$F(x) = \Pr(X \leq x)$$

The cdf is a function that returns *cumulative* probabilities, i.e. the probability that a random variable is smaller or equal to some fixed value x. The cdf can also be used to compute probabilities for intervals, since

$$\Pr(a \leq X \leq b) = \Pr(X \leq b) - \Pr(X \leq a) = F(b) - F(a).$$

Such probabilities can also be computed by integrating a so called **probability density function** or **pdf** for short.

probability density function

pdf

Definition. *The probability density function (pdf) for a random variable X is function $f(x)$ with properties*

- $f(x) \geq 0$ *for all* $-\infty < x < \infty$
- $\int_{-\infty}^{\infty} f(x)\mathrm{d}x = 1$
- $\Pr(a \leq X \leq b) = \int_a^b f(x)\,\mathrm{d}x$

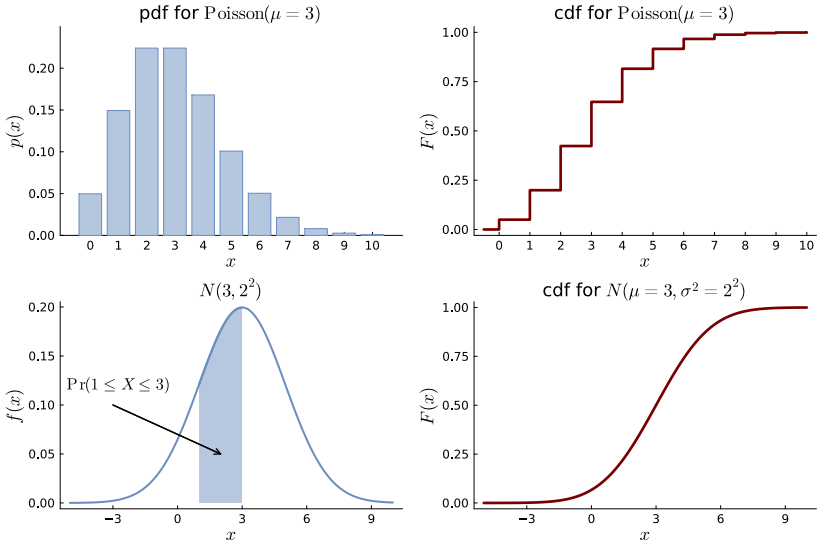

Figure 4.1: The poisson probability function (top left) and corresponding cumulative distribution function (top right). A normal probability density function is plotted in the bottom left and its cumulative distribution function is shown in the bottom right.

There is an intimate connection between the cdf and pdf: the pdf is the derivative of the cdf:

$$\frac{\mathrm{d}}{\mathrm{d}x}F(x) = f(x)$$

and conversely, the cdf is the integral of the pdf:

$$F(x) = \int_{-\infty}^{x} f(t)dt,$$

where we have used t as the integration variable instead of the usual x, to not confuse it with the upper limit of integration, which is x here. Recall that the integration variable is really just a dummy variable that can be given any symbol we like; I could have used y or z instead.

Example: Let the X be a random variable with probability density

function

$$f(x) = \begin{cases} 3x^2 & \text{for } 0 \leq x \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

This has the property of a pdf since is is non-negative and it integrates to one:

$$\int_{-\infty}^{\infty} f(x)dx = \int_0^1 3x^2\,\mathrm{d}x = [x^3]_0^1 = 1^3 - 0^3 = 1.$$

The cdf is obtained by integrating the pdf up to x

$$F(x) = \int_{-\infty}^{x} f(t)dt = \int_0^x 3t^2 dt = [t^3]_0^x = x^3.$$

The pdf is indeed the derivative of the cdf:

$$\frac{\mathrm{d}}{\mathrm{d}x}F(x) = \frac{\mathrm{d}}{\mathrm{d}x}x^3 = 3x^2.$$

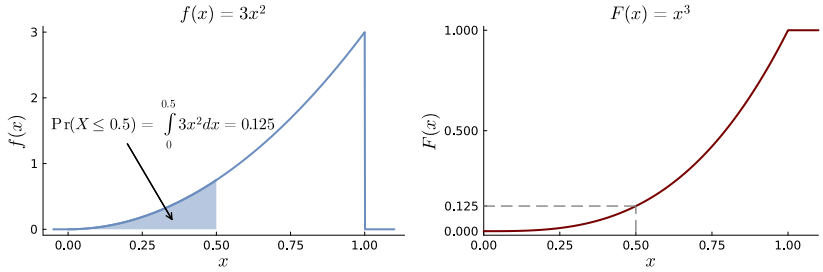

Figure 4.2: caption

4.2 *The expected value, median and variance*

It is often useful to summarize a random variable with a few numbers that aims to capture the shape of the distribution, for example the *location* and *spread*. This section introduces the most common location summaries for a random variable: the mean, mode and median, and also the variance and standard deviation to measure the spread of a distribution.

Definition. *The mean of a continuous random variable X is defined as*

$$\mathbb{E}(X) = \int_{-\infty}^{\infty} x \cdot f(x)dx$$

Example: The mean in the density $f(x) = 3x^2$ for $0 \leq x \leq 1$ is

$$\mu = \mathbb{E}(X) = \int_{-\infty}^{\infty} x \cdot 3x^2 dx = \int_0^1 3x^3 dx = \left[\frac{3}{4}x^4\right]_0^1 = \frac{3}{4}.$$

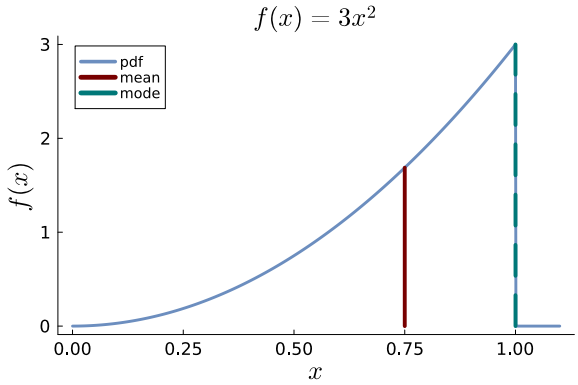

Figure 4.3: The mean of the density $f(x) = 3x^2$.

The mean is plotted as the red line in Figure 4.3.

The **mode**, mode(X) of a random variable is the value with highest density

mode

$$\text{mode}(X) = \arg\max_{x \in \mathcal{X}} f(x)$$

in the continuous case, or largest probability in the case with a discrete variable. The mode of the density $f(x) = 3x^2$ for $0 \leq x \leq 1$ is plotted as a green dashed line in the left graph of Figure 4.4; the mode happens to be at the boundary of the support here, mode$(X) = 1$.

An alternative summary of the location of a random variable is the median. The *median of a sample* $x_1, x_2, \ldots, x_n$ is the middle value when the data is sorted from the smallest to the largest observation. For example, the median of the data $2.1, 3.5, 1.9, 4.3, 2.7$ is 2.7. If n is even, the median can be defined as mean of the two observations in the middle. The median for a random variable is defined somewhat analogous to this middle observation idea. The *median of a continuous random variable*, med(X), is the smallest x that satisfies

$$F(x) = 0.5$$

That is, the median is the smallest value x that has exactly half of the probability mass to the left of x.

Example: Let X be a continuous random variable with density $f(x) = 3x^2$ for $0 \leq x \leq 1$. The cdf was derived earlier as $F(x) = x^3$. The median is obtained by solving the equation

$$F(x) = x^3 = 0.5$$

which has the solution $\text{med}(X) = (0.5)^{1/3} \approx 0.7944$. Figure 4.4 illustrates how the median (yellow dashed line) has half of the probability mass to the left of it. The median is larger than the mean (red line) in this example since it less affected by the long left tail with small

values. In general, the median is more *robust* to extreme values than the mean. This is why average income is most often reported as a median instead of a mean; otherwise a few extremely rich persons in the right tail of the income distribution would have a large effect on the average income. A common distribution for incomes is the LogNormal distribution presented later in Section 4.8, which is plotted in Figure 4.5. The distribution is skewed to the right (long tail on larger values) and the mean is clearly much more influenced by the probability mass in the right tail than the median and mode.

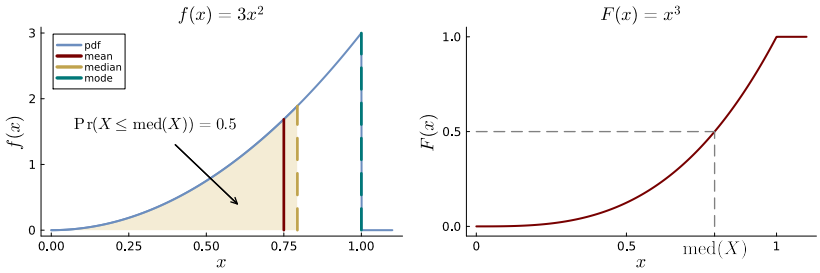

Figure 4.4: The graph to the left plots the median in the density $f(x) = 3x^2$ as a yellow dashed line, with half of the probability mass indicated by the yellow shaded area. The graph to the right plots the cdf $F(x) = x^3$ and the median as the smallest value that satisfies $F(x) = 0.5$.

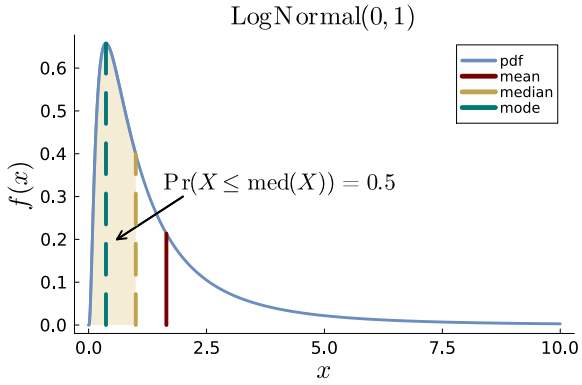

Figure 4.5: Illustration of the mean, median and mode in the standard log normal distribution.

For discrete random variables we are often not able to find an x that satifies the equation $F(x) = 0.5$, since the cdf may jump from one x to the next. See Figure 4.6 for an example where $\Pr(X \leq 1) = 0.25$ and $\Pr(X \leq 2) = 0.58$, so the median is somewhere between 1 and 2.

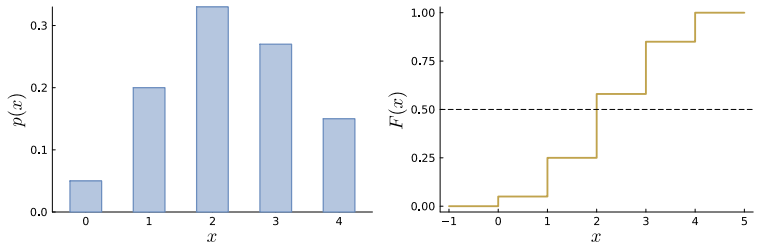

Figure 4.6: Illustrating that a discrete random variable may not have a median that satisfies $F(x) = 0.5$ since the cdf jumps at discrete values.

Definition. *The variance of a continuous random variable X is defined as*

$$\mathbb{V}(X) = \mathbb{E}(X)(X-\mu)^2 = \int_{-\infty}^{\infty} x \cdot f(x) dx$$

where $\mu = \mathbb{E}(X)$ is the mean of X.

Theorem 4.

$$\mathbb{V}(X) = \mathbb{E}(X^2) - \mu^2$$

where $\mu = \mathbb{E}(X)$ is the mean of X.

Proof.

$$\begin{aligned}\mathbb{V}(X) &= \mathbb{E}(X-\mu)^2 = \mathbb{E}(X^2 - 2\mu X + \mu^2) = \mathbb{E}(X^2) - 2\mu\mathbb{E}(X) + \mu^2 \\ &= \mathbb{E}(X^2) - 2\mu^2 + \mu^2 = \mathbb{E}(X^2) - \mu^2.\end{aligned}$$

□

EXAMPLE: The variance of a random variable with density $f(x) = 3x^2$ is

$$\mathbb{V}(X) = \mathbb{E}(X^2) - \mu^2,$$

where the expected value of X^2 is

$$\mathbb{E}(X^2) = \int_{-\infty}^{\infty} x^2 \cdot 3x^2 \, \mathrm{d}x = \int_{-\infty}^{\infty} 3x^4 \, \mathrm{d}x = \left[\frac{3}{5}x^5\right]_0^1 = \frac{3}{5}$$

so the variance is

$$\mathbb{V}(X) = \mathbb{E}(X^2) - \mu^2 = \frac{3}{5} - \left(\frac{3}{4}\right)^2 \approx 0.0375.$$

4.3 *Uniform distribution*

4.4 *Normal distribution*

4.5 *Exponential distribution*

To show the exponential distribution in action, we fit the model iid Exponential model $X_1, X_2, \ldots, X_n \overset{iid}{\sim} \text{Expon}(\beta)$ to the final price in $n = 862$ eBay coin auctions that attracted at least one bid. We use the maximum likelihood estimation method to find an optimal estimate $\hat{\beta}$ of the model parameter β; this estimator will be shown to be the sample mean $\bar{x}$ for the exponential model, which for this dataset is $\hat{\beta} = \bar{x} = 22.6$. A histogram of the data and the pdf of the fitted

Uniform distribution

$$X \sim \text{Unif}(a, b), \text{ with support } X \in (a, b)$$

Probability density function

$$f(x) = \frac{1}{b-a}$$

Expected value

$$\mathbb{E}(X) = \frac{a+b}{2}$$

Variance

$$\mathbb{V}(X) = \frac{(b-a)^2}{12}$$

Figure 4.7: Properties of the Uniform distribution.

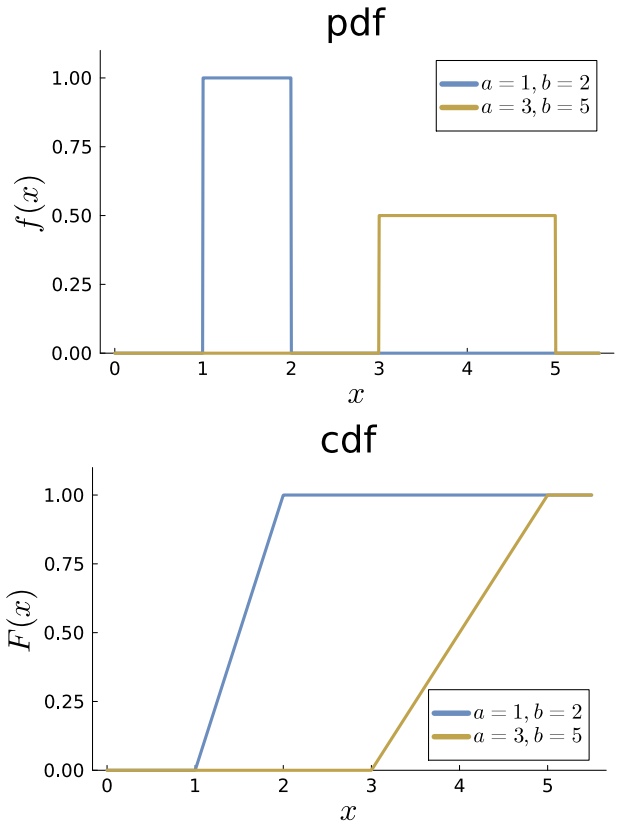

Figure 4.8: The Uniform distribution $\text{Unif}(a, b)$ pdf (top) and cdf (bottom) for some parameter values.

Normal distribution

$$X \sim N(\mu, \sigma^2), \text{ with support } X \in (-\infty, \infty)$$

Probability density function

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$$

Expected value

$$\mathbb{E}(X) = \mu$$

Variance

$$\mathbb{V}(X) = \sigma^2$$

Figure 4.9: Properties of the Normal distribution.

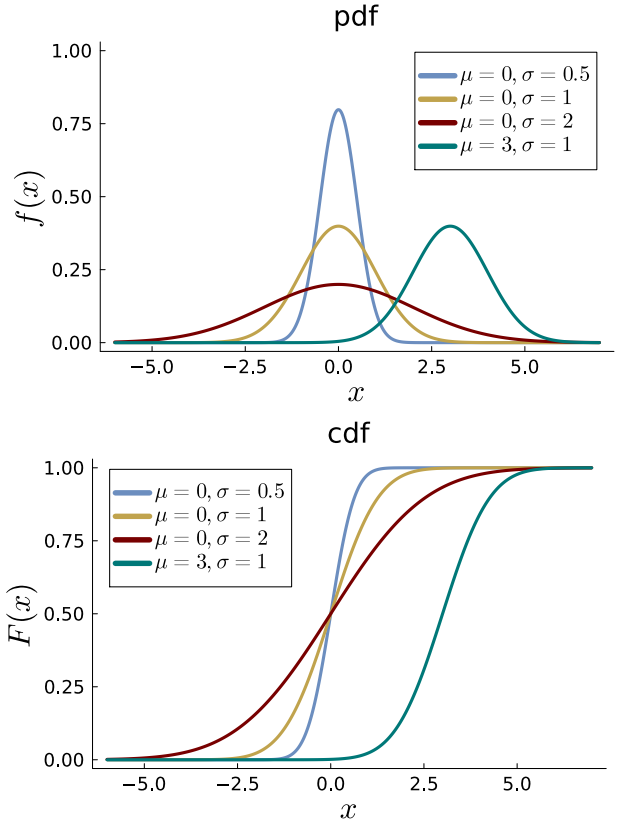

Figure 4.10: The normal distribution $N(\mu, \sigma^2)$ pdf (top) and cdf (bottom) for some parameter values.

Exponential distribution

$$X \sim \text{Expon}(\beta), \text{ with support } X \in (0, \infty)$$

Probability density function

$$f(x) = \frac{1}{\beta} e^{-x/\beta}$$

Expected value

$$\mathbb{E}(X) = \beta$$

Variance

$$\mathbb{V}(X) = \beta^2$$

Figure 4.11: Properties of the exponential distribution.

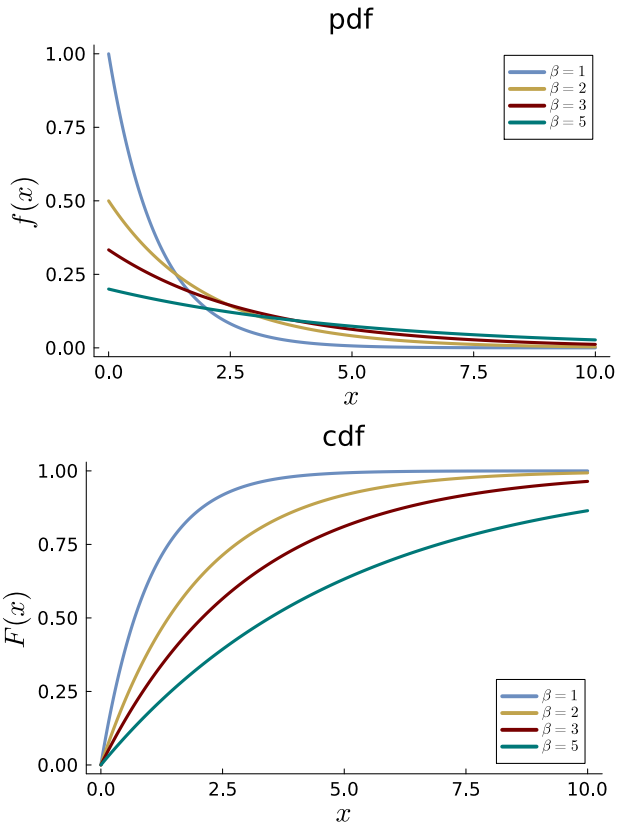

Figure 4.12: The exponential distribution Expon(β) pdf (top) and cdf (bottom) for some parameter values.

model is shown in the left hand graph of Figure 4.8. The empirical cdf and the fitted cdf is shown in the right hand graph. The monotonically decaying pdf of the exponential model is not able to capture what appear from the histogram to be data distribution with a mode slightly larger than zero. The histogram also reveals some large final prices, clearly in excess of 100; more precisely, around 2.6% of the final prices are larger than 100. To see how well the iid exponential model is able to capture this aspect of the data we compute that the fitted model implies $\Pr(X > 100) \approx 0.012$, which is less than half of the proportion observed in the data.

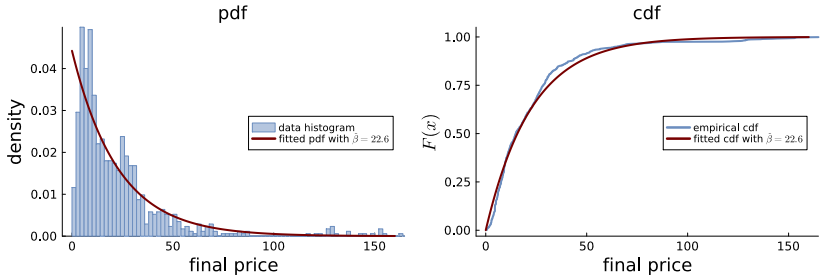

Figure 4.13: Fitting an exponential distribution to the final price in $n = 862$ eBay auctions. The fitted pdf (red) is shown to the left and the fitted cdf (red) to the right.

4.6 *Gamma distribution*

The Gamma distribution is a generalization of the exponential distribution for positive continuous random variables, for example suitable for modeling lifetime, income and waiting time data. The properties of the Gamma distribution are summarized in Figure .

Gamma distribution

$$X \sim \text{Gamma}(\alpha, \beta), \text{ with support } X \in (0, \infty)$$

Probability density function

$$f(x) = \frac{1}{\Gamma(\alpha)\beta^{\alpha}} x^{\alpha-1} e^{-x/\beta}$$

Expected value

$$\mathbb{E}(X) = \alpha\beta$$

Variance

$$\mathbb{V}(X) = \alpha\beta^2$$

Figure 4.14: Properties of the Gamma distribution.

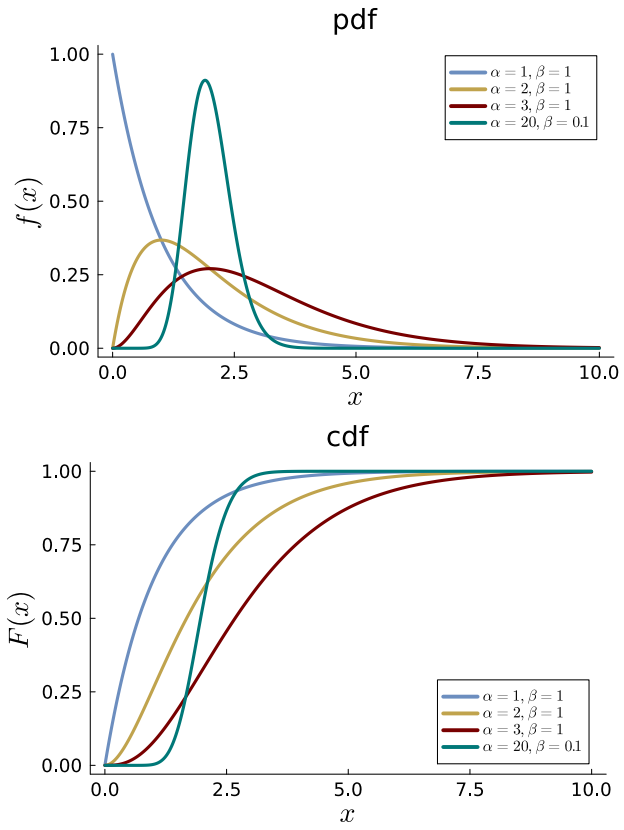

Figure 4.15: The Gamma distribution Gamma(α, β) pdf (top) and cdf (bottom) for some parameter values.

The relation to the exponential distribution is that the sum of independent Expon(β) variables follows a Gamma distribution:

$$\text{If } X_1, X_2, \ldots, X_\alpha \overset{\text{iid}}{\sim} \text{Expon}(\beta) \text{ then } \sum_{i=1}^{\alpha} X_i \sim \text{Gamma}(\alpha, \beta)$$

The Gamma distribution is fitted to the final price in the eBay coin auction data using the maximum likelihood estimator for the model parameters α and β. The estimates are $\hat{\alpha} = 1.260$ and $\hat{\beta} = 17.930$; note that the estimated α is not far from the value $\alpha = 1$ corresponding to the Exponential distribution. However, this seemingly small difference in α gives a fitted Gamma distribution that seems to better capture the mode of the histogram than the monotonoically decaying pdf from the exponential model; the fitted density near the mode is still too low however. Moreover, the Gamma model is not able to capture the extreme prices in the data since $\Pr(X > 100) \approx 0.0068$, which should be compared to 2.6% of observations larger than 100 in the data. The exponential model actually does a better job here.

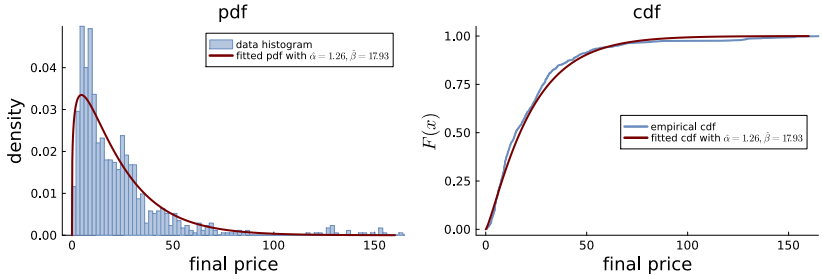

Figure 4.16: Fitting a Gamma distribution to the final price in $n = 862$ eBay auctions. The fitted pdf (red) is shown to the left and the fitted cdf (red) to the right.

4.7 *Chi-squared distribution*

chi-squared distribution

The **chi-squared distribution** is the special case of a Gamma distribution with parameters $\alpha = \nu/2$ and $\beta = 2$. The chi-squared distribution has a single parameter $\nu > 0$ which is called the *degrees of freedom*. Figure 4.17 gives the density and some properties and Figure 4.18 plots the chi-squared pdf and cdf for some values of the parameter ν.

The importance of the chi-squared distributions is its relation to the distribution of squared normal variable. In Section 6.1 we will derive the following result:

$$\text{If } X \sim N(0,1), \text{ then } X^2 \sim \chi^2(\nu = 1).$$

Hence, squaring a standard normal variable gives a new random variable $Y = X^2$ which follows a chi-squared distribution with one

Chi-squared distribution

$$X \sim \chi^2(\nu), \text{ with support } X \in (0, \infty)$$

Probability density function

$$f(x) = \frac{1}{2^{\nu/2}\Gamma(\nu/2)\beta^{\alpha}} x^{\nu/2-1} e^{-x/2}$$

Expected value

$$\mathbb{E}(X) = \nu$$

Variance

$$\mathbb{V}(X) = 2\nu$$

Figure 4.17: Properties of the chi-squared distribution.

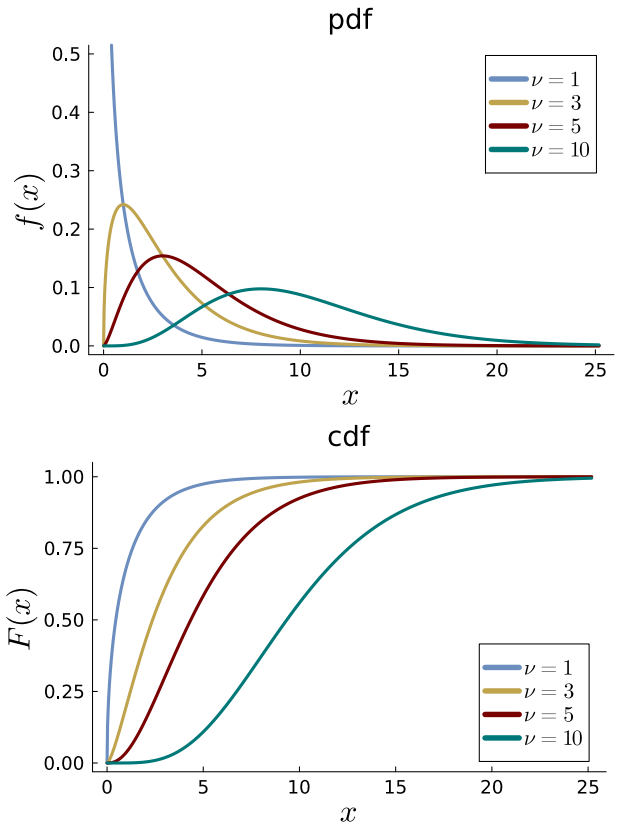

Figure 4.18: The Chi-squared distribution $\chi^2(\nu)$ pdf (top) and cdf (bottom) for some parameter values.

degree of freedom. One can also show that a sum of chi-squared variables also follows a chi-squared distribution:

$$\text{If } X_1, X_2, \ldots, X_\nu \overset{\text{iid}}{\sim} \chi^2(1) \text{ then } \sum_{i=1}^{\nu} X_i^2 \sim \chi^2(\nu),$$

so the sum of ν chi-squared variables, each with one degree of freedom, follows a chi-squared with ν degrees of freedom. Putting the above two results together, we have the following relation between the $\chi^2(\nu)$ distribution and the normal distribution:

$$\text{If } X_1, X_2, \ldots, X_n \overset{\text{iid}}{\sim} N(\mu, \sigma^2), \text{ then } \sum_{i=1}^{n} \left(\frac{X_i - \mu}{\sigma}\right)^2 \sim \chi^2(n).$$

since the standardized normal variables $Z_i = \frac{X_i - \mu}{\sigma}$ follow a $N(0,1)$ distribution. This result is important since it can be used to show that the sample variance

$$S^2 = \sum_{i=1}^{n} \frac{(X_i - \widehat{X})^2}{n-1}$$

follows a (scaled) chi-squared distribution.

4.8 *LogNormal distribution*

The LogNormal distribution is another distribution for positive continuous random variables. The LogNormal variable is the exponential of a normal random variable: The relation to the exponential distribution is that the sum of independent Expon(β) variables follows a Gamma distribution:

$$X \sim N(\mu, \sigma^2) \implies \exp(X) \sim \text{LogNormal}(\mu, \sigma^2)$$

The properties of the LogNormal distribution are summarized in Figure 4.19. Note that the parameters μ and σ^2 are not the mean and variance for a LogNormal variable, they are the mean and variance of the normal variable which is exponentiated to get the LogNormal variable. Figure 4.19 also gives the median since it often used in the context of LogNormal variables by virtue of it being more robust to extreme values than the mean, which is important for the LogNormal distribution since it is typically heavily skewed to the right. Figure shows that the LogNormal distribution seems to be a better fit to the eBay price data than the Exponential and Gamma distributions in Figures and , although the outliers in the right tail are still hard to catch with a sizeable probability.

Figure shows the iid LogNormal model fitted to the final price in the eBay coin auction data. The fit is a lot better than the Exponential and Gamma models. The LogNormal model also captures the extreme final prices well: the implied model probability of $\Pr(X > 100) \approx 0.024$ agrees with the 2.6% observed in the data.

LogNormal distribution

$$X \sim \text{LogNormal}(\mu, \sigma^2), \text{ with support } X \in (0, \infty)$$

Probability density function

$$f(x) =$$

Expected value

$$\mathbb{E}(X) = \exp\left(\mu + \frac{\sigma^2}{2}\right)$$

Variance

$$\mathbb{V}(X) = \left(\exp(\sigma^2) - 1\right)\exp(2\mu + \sigma^2)$$

Median

$$\text{med}(X) = \exp(\mu)$$

Figure 4.19: Properties of the LogNormal distribution.

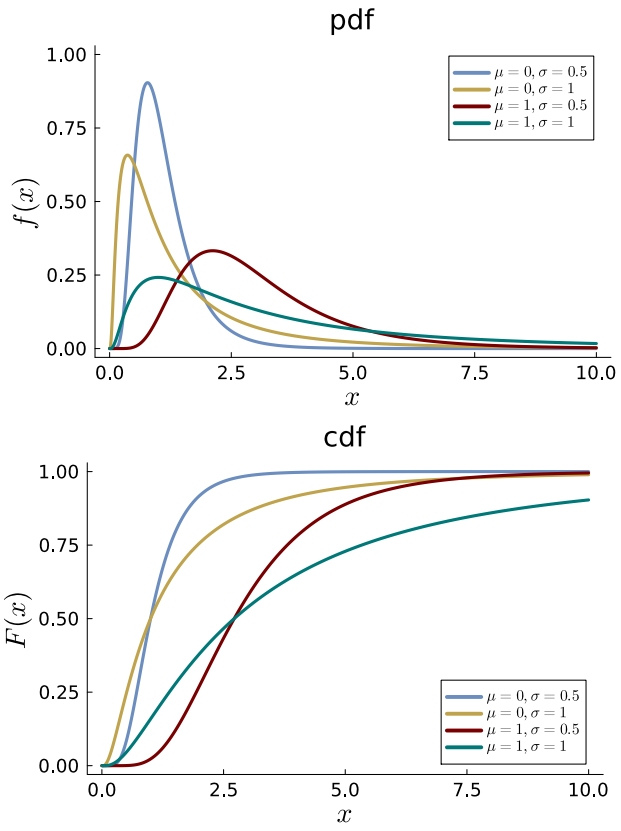

Figure 4.20: The LogNormal(μ, σ^2) pdf (top) and cdf (bottom) for some parameter values.

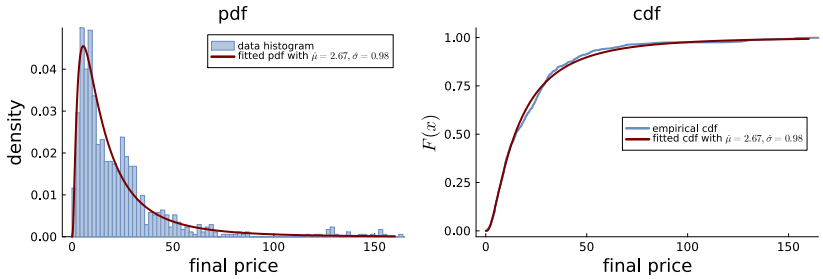

Figure 4.21: Fitting a LogNormal distribution to the final price in $n = 862$ eBay auctions. The fitted pdf (red) is shown to the left and the fitted cdf (red) to the right.

4.9 *Beta distribution*

Beta distribution

$$X \sim \text{Beta}(\alpha, \beta), \text{ with support } X \in (0, 1)$$

Probability density function

$$f(x) = \frac{1}{\text{Beta}(\alpha, \beta)} x^{\alpha-1}(1-x)^{\beta-1}$$

Expected value

$$\mathbb{E}(X) = \frac{\alpha}{\alpha + \beta}$$

Variance

$$\mathbb{V}(X) = \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$$

Figure 4.22: Properties of the Beta distribution.

Figure shows the fit of the Beta distribution to the nitrogen proportion in $n = 114$ balsam fir trees; see Geissinger et al. (2022) for a description of the data. The fitted pdf and cdf are shown in the left and right panels, respectively.

4.10 *Student-t distribution*

The student-t distribution is a probability distribution for continuous data that is symmetric and bell-shaped, like the normal distribution, but has heavier tails. The heavier tails means that the student-t distribution has more probability mass on extreme values, which can be useful in many settings.

Introductory courses in statistics usually only presented the distribution in its standard form, $t(\nu)$, with a location of zero, a scale of one and a single parameter ν called the *degrees of freedom* to model the tails of the distribution. The usual application of the standard

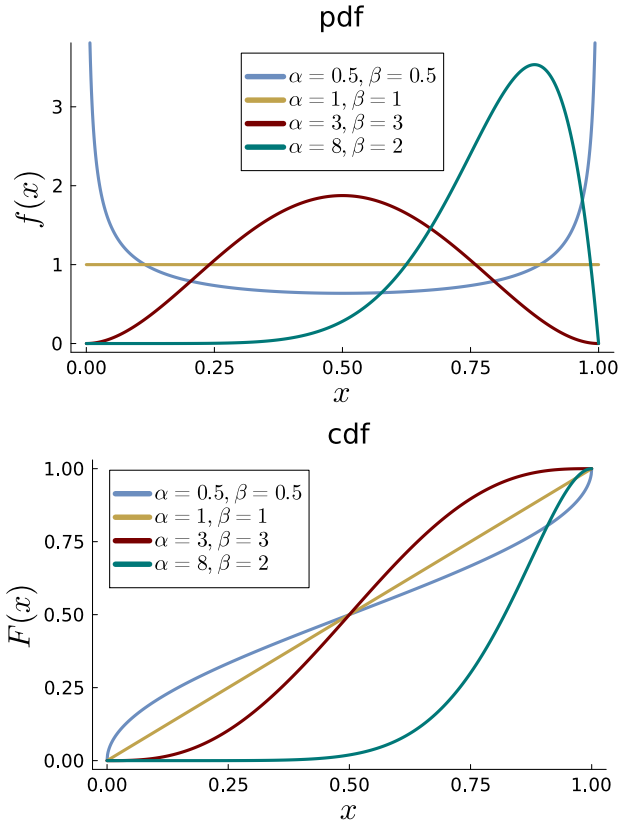

Figure 4.23: The beta distribution Beta(α, β) pdf (top) and cdf (bottom) for some parameter values.

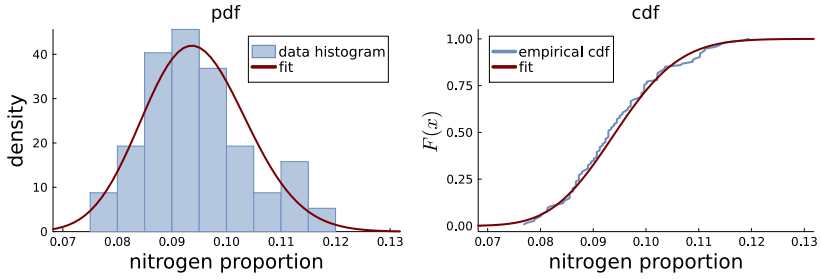

Figure 4.24: Fitting a Beta distribution to nitrogen proportion in $n = 114$ balsam fir trees. The fitted pdf (red) is shown to the left and the fitted cdf (red) to the right.

student-t distribution is to model the distribution of a standardized sample mean when the population variance is unknown.

Our interest here is instead in using the student-t distribution as a model for heavy-tailed data, and we will therefore use the more general three-parameter version of the student-t distribution: $t(\mu, \sigma, \nu)$, where μ is the location parameter, σ is the scale parameter and ν is the **degrees of freedom**. The parameter ν controls how heavy the tails are: lower values give heavier tails and as $\nu \to \infty$, the student-t distribution becomes the normal distribution; see Section 5.2. Note also that ν is allowed to be any positive real number, not just an integer as it is usually presented in connection to the sample mean where $\nu = n - 1$ happens to be an integer. The properties of the student-t distribution are summarized in Figure 4.25, and the pdf and cdf are plotted in Figure 4.26 for some combinations of parameter values.

degrees of freedom

Student-t distribution

$$X \sim t(\mu, \sigma, \nu), \text{ with support } X \in (-\infty, \infty)$$

Probability density function

$$f(x) = \frac{\Gamma((\nu+1)/2)}{\Gamma(\nu/2)\sqrt{\pi\nu\sigma^2}} \cdot \left(1 + \frac{1}{\nu}\left(\frac{x-\mu}{\sigma}\right)^2\right)^{-(\nu+1)/2}$$

Expected value

$$\mathbb{E}(X) = \mu \text{ if } \nu > 1$$

Variance

$$\mathbb{V}(X) = \sigma^2 \frac{\nu}{\nu - 2} \text{ if } \nu > 2$$

Figure 4.25: Properties of the Student-t distribution.

Figure 4.27 shows the fit of a student-t distribution to daily returns on the Ericsson stock during $n = 252$ the trading days in the year 2022. The student-t distribution is here fitted under the iid assumption, which is not likely to hold here since the data is a time series, which typically has dependent observation. The Bayesian Learning book presents more sophisticated stochastic volatility models for time series with heavy-tailed observations, but we will here continue with the simplistic iid assumption for illustration. The parameters are estimated with the maximum likelihood method presented in Chapter 8. The fitted pdf and cdf in Figure 4.27 are shown as red lines in the left and right panels, respectively. The maximum likelihood estimates of the parameters for the student-t distribution are $\mu = -0.094$, $\sigma = 1.279$ and $\nu = 2.706$. The fit from a normal distribution is shown in blue as a reference. The student-t distribution clearly fits the data

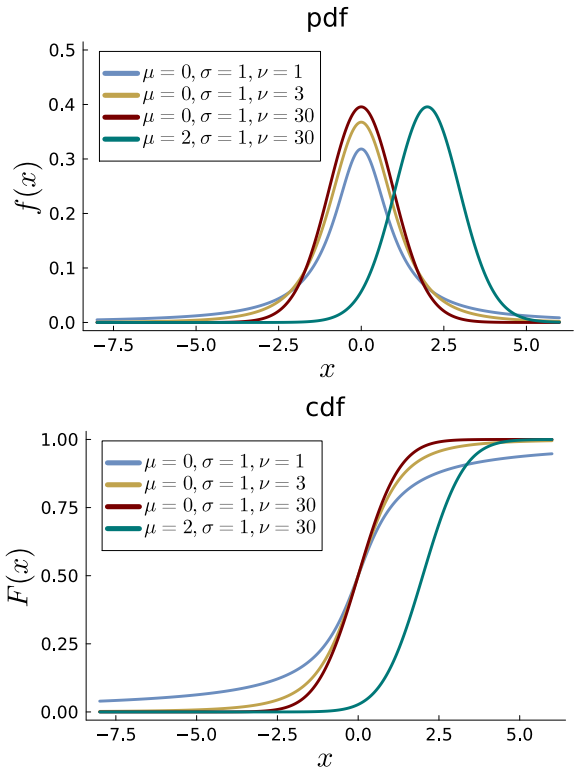

Figure 4.26: The student-t distribution $t(\mu, \sigma, \nu)$ pdf (top) and cdf (bottom) for some parameter values.

much better than the normal distribution, which is not surprising since stock market returns data tend to be heavy-tailed. In an attempt to catch the heavy tails of the data, the estimate variance parameter σ is the normal distribution is inflated, leading to a rather poor fit of the center of the data distribution. The degrees of freedom parameter ν is estimated to a low value of $\nu = 2.706$, which is another indication of the heavy tails of the data.

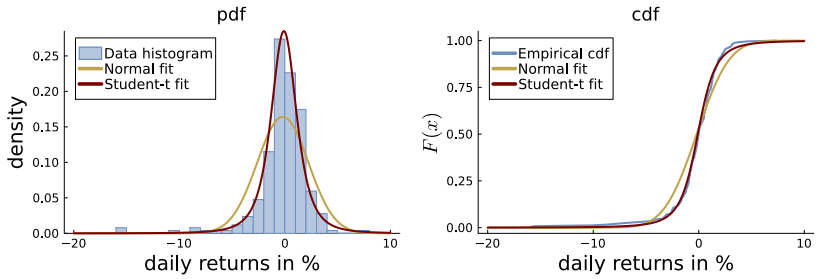

Figure 4.27: Fitting a student-t distribution to $n = 252$ daily returns on the Ericsson stock. The fitted student-t pdf (red) is shown to the left and the fitted student-t cdf (red) to the right. The best fitting normal distribution is shown in blue.

Let us explore the issue of the tails of a distribution a bit more. The pdf curves in left graph of Figure 4.23 shows that the student-t distribution with lower degrees of freedom have more probability mass in the tails, but it is hard to appreciate from a plot of the pdf

just how much effect this has. A plot of *logarithm* of the pdf gives more insights. The left graph in Figure 4.28 shows the logarithm of the pdf for different values of ν and the logarithm of the pdf for the normal distribution as a reference. The tails of the log pdf of the normal distribution decay fast to zero in a quadratic fashion while the student-t distribution has a much slower decay, even slower than linear for small values of ν.

Another way to explore the tail behavior of a distribution is to look at the distribution of the *maximal* observation

$$X_{\max} = \max\{X_1, \ldots, X_n\}$$

in a sample of size n; the maximum of a sample is also called the **largest order statistic**. The idea is that a heavy-tailed distribution is more likely to produce extreme values than a light-tailed distribution. The right graph in Figure 4.28 shows the pdf for the maximum observation $X_{\max}$ in a sample of size $n = 50$ for different values of ν. If the data are from $N(0,1)$ it is nearly impossible to get a maximum of more than $x_{\max} = 5$ (the probability is 0.000014), but quite probable if the data are from a student-t with three degrees of freedom (the probability is 0.320). The variance of the student-t with three degrees is $\frac{\nu}{\nu-2} = 3$, so maybe a more fair comparison is between the student-t with three degrees and the $N(0,3)$ distribution. But also with this modification, the probability for $X_{\max} \geq 5$ is only 0.09 for the normal distribution. The distribution of the maximum may seem like a complicated calculation, but it turns out to be quite simple; the result is given in Theorem 4.10 below, for any continuous distribution.

largest order statistic

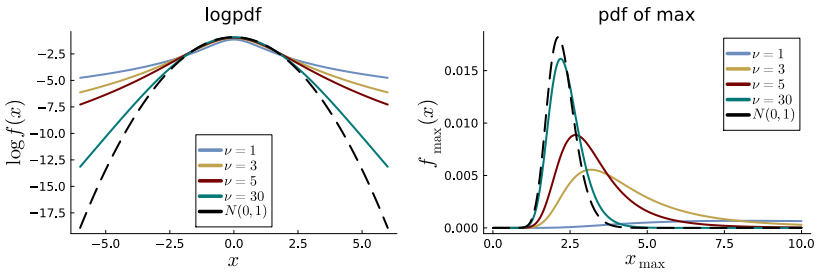

Figure 4.28: Illustration of the heavy tails of the student-t distribution. The left panel shows the logarithm of the pdf for different values of ν. The right panel shows the pdf for the largest observation $x_{\max}$ in a sample of $n = 50$ observations for different values of ν. The dashed line shows the pdf for the normal distribution (corresponding to $\nu \to \infty$) as a reference.

Theorem 5. ***(Distribution of the maximum of sample)*** *Let $X_1, \ldots, X_n$ be iid continuous random variables with density $f(x)$ and distribution function $F(x)$. Let*

$$X_{\max} = \max(X_1, \ldots, X_n)$$

be the maximum of a sample of size n. The pdf of the maximum is then

$$f_{\max}(x_{\max}) = nf(x_{\max})\big(F(x_{\max})\big)^{n-1}$$

Proof. The maximum of a sample $X_{\max}$ is smaller than or equal to some value $x_{\max}$ if and only if all observations are smaller than or equal to $x_{\max}$. Hence

$$\begin{aligned} F_{\max}(x_{\max}) &= \Pr(X_{\max} \leq x_{\max}) = \Pr(X_1 \leq x_{\max}, \ldots, X_n \leq x_{\max}) \\ &= \Pr(X_1 \leq x_{\max}) \cdots \Pr(X_n \leq x_{\max}) \\ &= \big(F(x_{\max})\big)^n, \end{aligned}$$

where we have used the fact that the observations are independent so that the joint probability is the product of the individual probabilities and that the cdf is the same $F(x)$ for all observations. The probability density function for the maximum is then given by the derivative of the cumulative distribution function:

$$\begin{aligned} f_{\max}(x_{\max}) &= \frac{\mathrm{d}}{\mathrm{d}x_{\max}} F_{\max}(x_{\max}) = \frac{\mathrm{d}}{\mathrm{d}x_{\max}} \big(F(x_{\max})\big)^n \\ &= n\big(F(x_{\max})\big)^{n-1} f(x_{\max}), \end{aligned}$$

using the chain rule to compute the derivative. □

5 Convergence and the central theorems

This chapter will introduce concepts of convergence of random variables. These ideas will be lead up to two of the most fundamental results in statistics concerning the distribution of the sample mean in large samples. We will learn that the sample mean of independent random variables will get closer and closer to the population mean (the *law of large numbers*), and also that the sample mean will be close to a normal distribution in large samples, regardless of which distribution that data came from (the *central limit theorem*).

5.1 Markov's and Chebyshev's inequalities

We first present **Markov's inequality**, which will be used to prove the Chebyshev's inequality later in this section.

Markov's inequality

Lemma. *For any non-negative random variable Y and any constant $a > 0$, we have*

$$\Pr(Y \geq a) \leq \frac{\mathbb{E}(Y)}{a} \tag{5.1}$$

Proof. We have

$$\begin{aligned}\mathbb{E}(Y) &= \int_0^\infty y f(y)\,\mathrm{d}y = \int_0^a y f(y)\,\mathrm{d}y + \int_a^\infty y f(y)\,\mathrm{d}y \\ &\geq \int_a^\infty y f(y)\,\mathrm{d}y \geq \int_a^\infty a \cdot f(y)\,\mathrm{d}y = a\int_a^\infty f(y)\,\mathrm{d}y \\ &= a \cdot \Pr(Y \geq a)\end{aligned}$$

where the first inequality uses that $\int_0^a y f(y)\,\mathrm{d}y > 0$, since y is always positive in the integral and $f(y) \geq 0$. Dividing both sides by a proves the result. □

Chebyshev's inequality gives an upper bound on the probability that a random variable deviates by at least k standard deviation from its mean, *regardless of the distribution of the random variable* That is, it provides a conservative value that is guaranteed to be larger than the

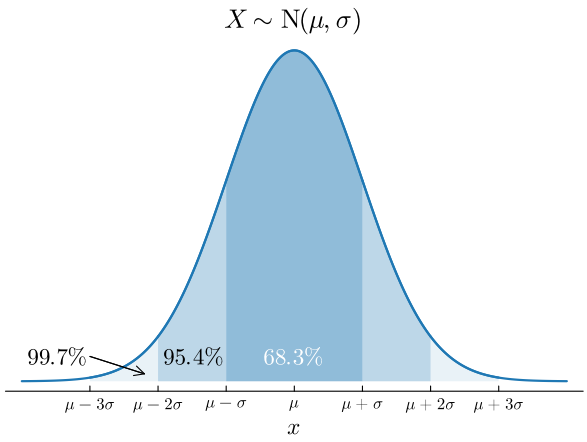

Figure 5.1: The normal interval rule. The left figure shows the probability of being within 1σ, 2σ and 3σ of the mean for a normal distribution. The right figure shows the same for the standard normal distribution.

actual probability of the event

$$\Pr(|X - \mu| \geq k\sigma).$$

For a normal distribution, the probability of deviating more than 2 standard deviations from the mean is 0.0455; see Figure 5.1. For the t-distribution with 3 degrees of freedom the same event has probability 0.0405. The probability of deviating more than 3 standard deviations from the mean is 0.0027 for the normal distribution and 0.0138 for the t-distribution with 3 degrees of freedom. The blue (normal) and red (t-distribution) curves in Figure 5.2 show these probabilities $\Pr(|X - \mu| \geq k\sigma)$ as a function of the number of standard deviations from the mean, k.

Chebyshev's inequality

Chebyshev's inequality in Theorem 5.1 gives a general bound on the probability of deviating more than k standard deviations from the mean. The bound holds for *all* distributions (with finite variance).

Theorem 6. *Let X be a random variable with mean μ and variance σ^2. Then, for any constant $k > 0$, we have*

$$\Pr(|X - \mu| \geq k\sigma) \leq \frac{1}{k^2}$$

Proof. Note first that

$$\Pr(|X - \mu| \geq k\sigma) = \Pr\Big((X - \mu)^2 \geq k^2\sigma^2\Big),$$

since the two set $\{x : |x - \mu| \geq k\sigma\}$ and $\{x : (x - \mu)^2 \geq k^2\sigma^2\}$ are the same. We now apply Markov's inequality to the positive random variable $Y = (X - \mu)^2$ and the constant $a = k^2\sigma^2$ to obtain

$$\Pr\Big((X - \mu)^2 \geq k^2\sigma^2\Big) \leq \frac{\mathbb{E}((X - \mu)^2)}{k^2\sigma^2} = \frac{\sigma^2}{k^2\sigma^2} = \frac{1}{k^2}.$$

which proves the result. □

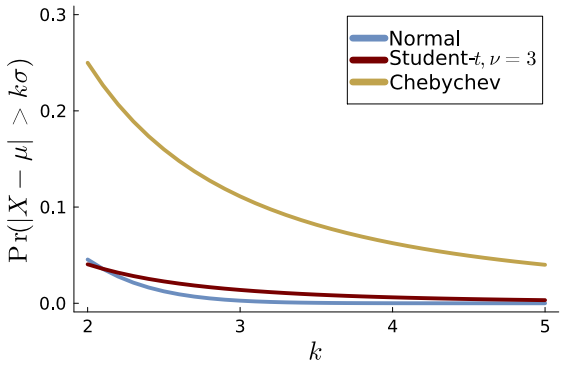

Figure 5.2: The Chebychev bound on the probability $\Pr(|X - \mu| \geq k\sigma)$ for different k compared to actual probabilities for two distributions.

The generality of Chebyshev's inequality has the drawback that the bound $\frac{1}{k^2}$ is usually much larger than the actual probability $\Pr(|X - \mu| \geq k\sigma)$, so the bound in the Theorem has very limited use for practical work. This is seen in Figure 5.2 where the yellow line plots the Chebyshev bound $\frac{1}{k^2}$, which is clearly much too large for all k for the normal and t(3) distributions. This observable widget explores the accuracy of the bound for some other distributions; the widget includes a three-point distribution where the bound is actually tight, which shows that the $\frac{1}{k^2}$ bound cannot be made smaller if we want to cover all possible distributions. The main use of Chebyshev's inequality is for mathematical proofs, and will later use the inequality to prove the law of large numbers in Section 5.3.

5.2 *Stochastic convergence*

In Chapter 1.12 we learned about the limit $L = \lim_{x \to a} f(x)$ of a mathematical function $f(x)$ as x approached a certain value a. One special case of that is limits at infinity $\lim_{x \to \infty} f(x)$. In Statistics we are often interested in how a statistical method performs in large samples, which is typically analyzed in an idealized setting where the sample size n approaches infinity. The situation with random variables is more complicated, however, since random variables can occasionally attain extreme values, even if the probability of such events may be low. We will therefore never be able to *guarantee* that $|X_n - L| < \epsilon$ with certainty for some sequences of random variables $X_1, \ldots, X_n$, but perhaps we can hope for the probability of this event going to zero as $n \to \infty$- Hence, we need a *probabilistic* concept of a limit, and notions of **stochastic convergence**. We will now introduce three different types of stochastic convergence: *convergence in probability*, *convergence in distribution* and *almost sure convergence*.

stochastic convergence

Convergence in probability

Consider a sequence of random variables $X_1, X_2, \ldots, X_n$. This could be the sequence of sample means $\bar{X}_n = \sum_{i=1}^{n} X_i$ or some other sequence. We are here interested in where this sequence ends up as n grows large, i.e. if X_n eventuelly converges to some fixed constant, in some sense, and, if so, which constant?

converges in probability

The sequence **converges in probability** to the constant c if the probability of the random variable being outside the interval $(c - \epsilon, c + \epsilon)$ goes to zero as n increases. This means that the distribution of X_n becomes more and more concentrated around the point c as n increases. Here is the definition.

Definition. *A sequence of random variables $X_1, \ldots, X_n$* ***converges in probability to a constant*** *c, if for all $\epsilon > 0$*

$$\Pr(|X_n - c| > \epsilon) \to 0 \quad \textit{as} \quad n \to \infty.$$

We then write $X_n \xrightarrow{p} c$.

Figure 5.3 illustrates the idea with convergence in probability of a sequence of random variables $X_1, X_2, \ldots, X_n$ to a constant c. The probability distribution for each X_n in the sequence is represented by the 50% (darker shaded region) and 95% (lighter shaded region) probability intervals. The region $(X - \epsilon, X + \epsilon)$ is marked out by a black horizontal line. The distribution of X_n becomes more and more concentrated around c as n increases, and the probability of being outside the interval $(X - \epsilon, X + \epsilon)$ goes to zero.

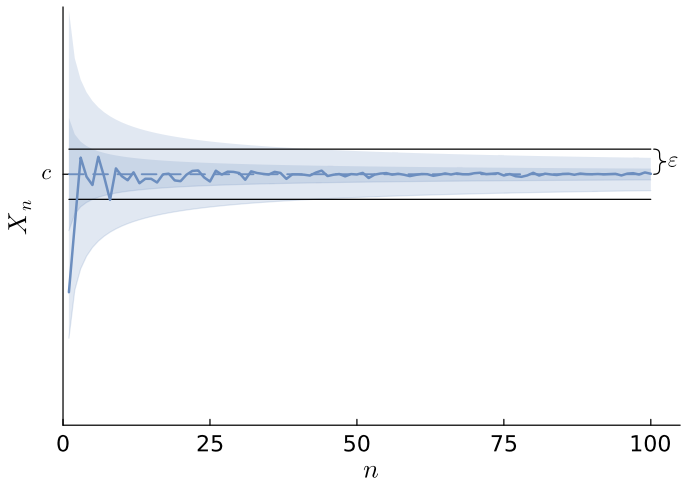

Figure 5.3: Illustrating convergence in probability of the sequence X_n to a constant c (horizontal dashed line) by plotting a realization of X_n for $n = 1, \ldots, 100$ (solid line). The probability distribution for each X_n in the sequence is represented by the 50% (darker shaded region) and 95% (lighter shaded region) probability intervals. The region $(X - \epsilon, X + \epsilon)$ is marked out by a black horizontal line. The distribution of X_n becomes more and more concentrated around c as n increases, and the probability of being outside the interval $(X - \epsilon, X + \epsilon)$ goes to zero.

EXAMPLE: Let $X_1, X_2, \ldots, X_n$ be an iid sample from $N(\mu, \sigma^2)$, then, as we showed in Section X, the sample mean follows a normal distribution

$$\bar{X}_n \sim N\Big(\mu, \frac{\sigma^2}{n}\Big).$$

Since the variance goes to zero as $n \to \infty$, the distribution of $\bar{X}_n$ becomes more and more concentrated around the mean μ in larger samples. It is then clear that for all $\epsilon > 0$ that

$$\Pr(|\bar{X}_n - \mu| > \epsilon) \to 0 \quad \text{as} \quad n \to \infty$$

and therefore than the sample mean converges in probability to the population mean μ; hence, $\bar{X}_n \xrightarrow{p} \mu$. This is a manifestation of the *law of large numbers* that generalizes this result to hold for the sample mean based on independent data from *any* distribution with finite variance, not just the normal distribution. Actaully, it even holds more generally without the requirement of a finite variance and also for certain forms of dependent data.

In the above definition of convergence in probability the sequence of random variables converged to a *constant*. We can also have convergence in probability toward a new *random variable*, as in the following definition.

Definition. *A sequence of random variables $X_1, \ldots, X_n$* ***converges in probability to a random variable*** *X if for all $\epsilon > 0$*

$$\Pr(|X_n - X| > \epsilon) \to 0 \quad \textit{as} \quad n \to \infty.$$

We write $X_n \xrightarrow{p} X$.

EXAMPLE: Define the sequence $X_n = X + \frac{1}{n}Y_n$, where $X \sim N(0,1)$ is a random variable and $Y_1, Y_2, \ldots \overset{\text{iid}}{\sim} N(0,1)$. Since $X_n - X = \frac{1}{n}Y_n \sim N\Big(0, \frac{1}{n}\Big)$ the distribution of $X_n - X$ becomes increasing concentrated over the point 0 and therefore $\Pr(|X_n - X| > \epsilon) \to 0 \quad \text{as} \quad n \to \infty$. Hence, $X_n \xrightarrow{p} X$. Figure X illustrates by plotting two realizations of X and of the sequence $X_n = X + \frac{1}{n}Y_n$; the probability distribution for each X_n is represented by the 50% (darker shaded regions) and 95% (lighter shaded regions) probability intervals.

Convergence in distribution

The second type of convergence is **convergence in distribution**. This type of convergence is weaker than convergence in probability, and is used to show that a sequence of random variables converges to a limiting distribution. Here is the definition.

convergence in distribution

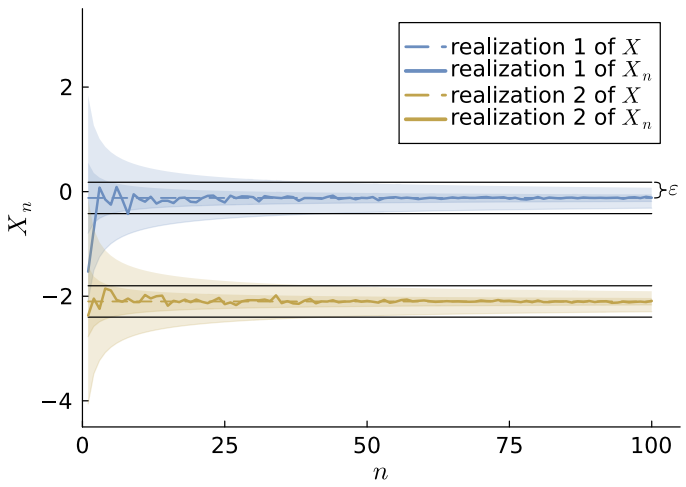

Figure 5.4: Illustrating convergence in probability of the sequence $X_n = X + \frac{1}{n}Y_n$ where $X \sim N(0,1)$ and and $Y_1, Y_2, \ldots \overset{\text{iid}}{\sim} N(0,1)$ by plotting two realizations of X (horizontal dashed lines) and the realized X_n sequence for $n = 1, \ldots, 100$ (solid lines). The probability distribution for each X_n is represented by the 50% (darker shaded regions) and 95% (lighter shaded regions) probability intervals. The region $(X - \epsilon, X + \epsilon)$ is marked out by black horizontal lines. Regardless of the realization, the distribution of X_n becomes more and more concentrated around X for each realization as n increases, and the probability of being outside the interval $(X - \epsilon, X + \epsilon)$ goes to zero.

Definition. *A sequence of random variables $X_1, \ldots, X_n$* ***converges in distribution*** *to the random variable X, if*

$$F_n(x) \to F(x) \quad as \quad n \to \infty,$$

for all x where $F(\cdot)$ is continuous, where $F_n(x)$ and $F(x)$ are the cumulative distribution functions (cdf) of X_n and X, respectively. We then write $X_n \xrightarrow{d} X$.

Example: The negative binomial distribution in the mean parameterization $\text{NegBin}(r, \mu)$ converges in distribution to the Poisson distribution $\text{Pois}(\mu)$ as $r \to \infty$. This is illustrated in Figure 5.5 where the top row shows the probability function (pdf), the middle row the cumulative distribution function (cdf) and the last row the difference in cdf between the negative binomial and Poisson distributions, for increasing values of r. We can write this symbolically as

$$\text{NegBin}(r, \mu) \xrightarrow{d} \text{Pois}(\mu) \quad \text{as} \quad r \to \infty.$$

Example: The student-t distribution with ν degrees of freedom converges in distribution to the standard normal distribution $N(0,1)$ as $\nu \to \infty$. This is illustrated in Figure 5.6, and we can write this symbolically as

$$\text{t}(\nu) \xrightarrow{d} N(0,1) \quad \text{as} \quad \nu \to \infty.$$

*Convergence almost surely**

Finally, we have the following definition of **almost sure convergence**.

almost sure convergence

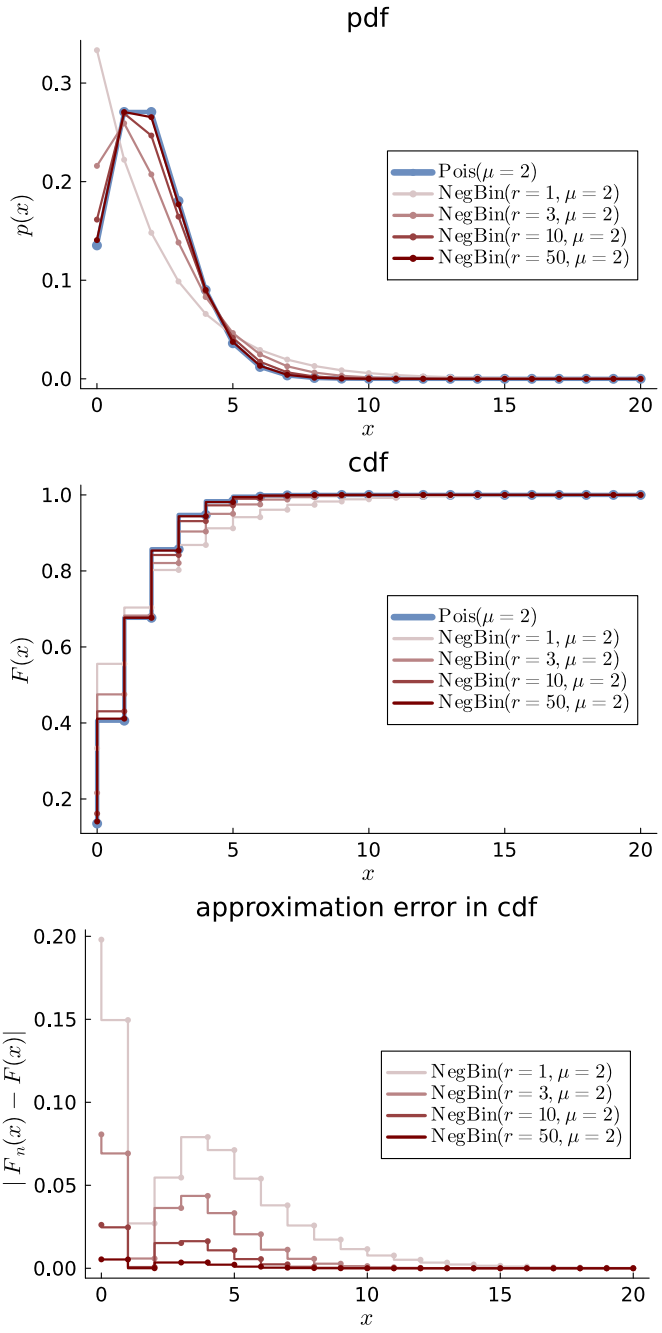

Figure 5.5: Illustration of how the NegBin(r, μ) converges in distribution to the Pois(μ) as $r \to \infty$. The top row shows the probability function (pdf), the middle row the cumulative distribution function (cdf) and the last row the difference in cdf between the negative binomial and Poisson distributions.

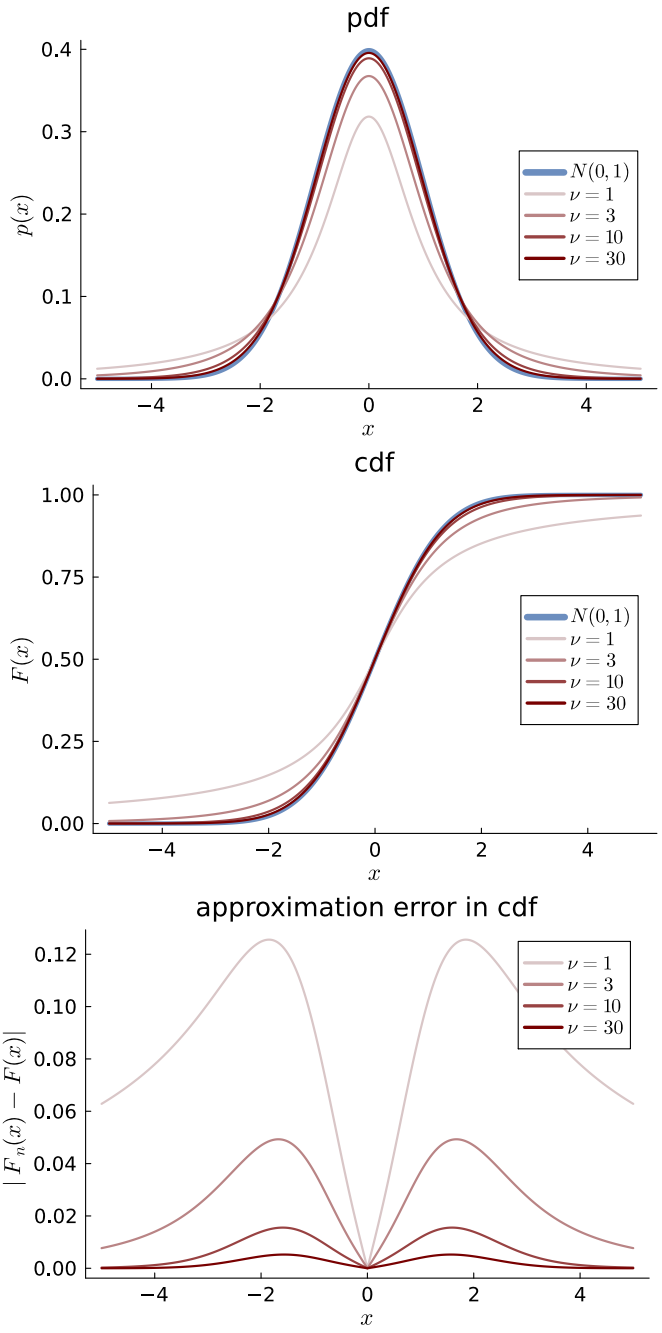

Figure 5.6: Illustration of how the student-t distribution with ν degrees of freedom converges in distribution to the $N(0,1)$ as $\nu \to \infty$. The top row shows the probability density function (pdf), the middle row the cumulative distribution function (cdf) and the last row the difference in cdf between the student-t and normal distributions.

Definition. *A sequence of random variables $X_1, \ldots, X_n$* ***converges almost surely to a random variable*** *X if*

$$\Pr(\lim_{n\to\infty} X_n = X) = 1$$

We write $X_n \xrightarrow{a.s.} X$.

Recall that a stochastic variable X is a function from the sample space Ω to the real numbers $\mathbb{R}$, so that $X(\omega)$ means the value of the random variable X for the outcome $\omega \in \Omega$. For example, Ω could be the set of all possible outcomes when rolling two dice, and $X(\omega)$ the sum of the dots on the two dice. Almost sure convergence can then be more clearly expressed as

$$\Pr\Big(\omega \in \Omega : \lim_{n\to\infty} X_n(\omega) = X(\omega)\Big) = 1$$

for all $\omega \in \Omega$. This means that the probability of the event where the sequence does not converge to X is zero.

Almost sure convergence is the strongest form of stochastic convergence among the three forms presented here. This means that if a sequence $X_1, \ldots, X_n$ of random variables converges almost surely to a random variable X, then the sequence also converges in probability and in distribution to that variable. In fact, the following relationships hold between the three types of convergence:

$$X_n \xrightarrow{a.s.} X \implies X_n \xrightarrow{p} X \implies X_n \xrightarrow{d} X.$$

Example: Consider the sequence

$$X_n \sim \begin{cases} N\left(0, \frac{1}{n}\right) & \text{with probability } \frac{n-1}{n} \\ N(0,1) & \text{with probability } \frac{1}{n} \end{cases}$$

Each random variable in the sequence is therefore a mixture of two normal distributions: one with a variance that decreases with n and one with a constant variance of 1 for all n; Figure 5.7 plots this distribution for some member of the sequence. The mixture probability on the density with constant variance is $\frac{1}{n}$ and therefore goes to zero as n increases.

To show that the sequence converges to zero in probability it is enough to show that the variance goes to zero with n. The law of total variance presented in Chapter 7 can be used to show that the variance is

$$\mathbb{V}(X_n) = \frac{1}{n}\Big(\frac{2n-1}{n}\Big)$$

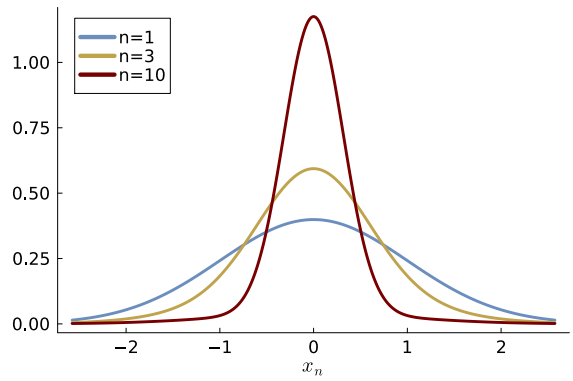

Figure 5.7: The mixture distributions for X_n for some n in the normal mixture example.

which goes to zero as n increases. So $X_n \xrightarrow{p} 0$.

However, the sequence does not converge almost surely to 0. To formally show this requires more probabilistic machinery than we have presented in this book; the lack of almost sure convergence comes from the probability for the normal distribution with constant variance, $\frac{1}{n}$, which goes to zero too slowly with n; there is always a small chance of the sequence taking a larger value from the normal distribution with constant variance, and this chance does not go to zero fast enough. Figure 5.8 illustrates the situation. For the convergence in probability we need that the probability mass of X_n gets concentrated in the interval $(-\epsilon, \epsilon)$, which is seen to be the case for large enough n. However, some realizations are still coming from the normal distribution with constant variance, even at large n, which is the reason why the sequence does not converge almost surely to 0.

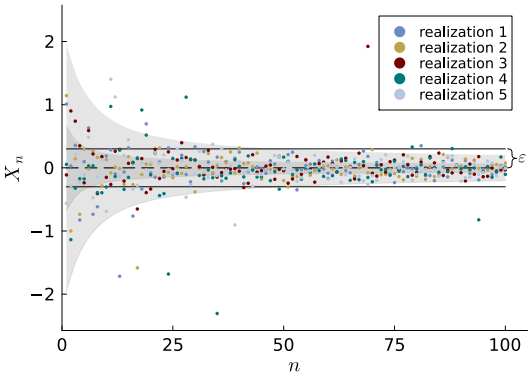

Figure 5.8: Contrasting almost sure convergence and convergence in probability in the mixture of normals example.

5.3 *Law of large numbers*

Define the sample mean as

$$\bar{X}_n := \frac{1}{n}\sum_{i=1}^{n} X_i, \tag{5.2}$$

so that the sample size appears explicity in the subscript. The **law of large numbers** say that the sample average $\bar{X}_n$ of independent random variables with mean $\mu = \mathbb{E}(X)$ is more and more probable to be close to the mean μ as the sample size grows large; we say that *the sample mean $\bar{X}_n$ converges to the population mean μ*. More formally, we have the following theorem.

law of large numbers

Theorem 7 (law of large numbers)**.**
For independent random variables $X_1, X_2, \ldots$ with finite mean $\mu = \mathbb{E}(X)$ and finite variance we have

$$\bar{X}_n \xrightarrow{p} \mu$$

where $\xrightarrow{p}$ denotes convergence in probability, i.e., for all $\epsilon > 0$

$$\Pr(|\bar{X}_n - \mu| \geq \epsilon) \to 0 \quad \textit{as} \quad n \to \infty \tag{5.3}$$

Proof. From the definition of convergence in probability, we need to prove that

$$\Pr\Big(|\bar{X}_n - \mu| \geq \varepsilon\Big) \to 0 \text{ as } n \to \infty$$

Recall that $\mathbb{E}(\bar{X}_n) = \mu$ and $\mathbb{S}(\bar{X}_n) = \frac{\sigma}{\sqrt{n}}$. Now, using Chebyshev's inequality with $k = \epsilon/(\frac{\sigma}{\sqrt{n}})$ we get

$$\Pr\Big(|\bar{X}_n - \mu| \geq \epsilon\Big) = \Pr\Big(|\bar{X}_n - \mu| \geq \frac{\epsilon}{\frac{\sigma}{\sqrt{n}}}\frac{\sigma}{\sqrt{n}}\Big) \leq \frac{1}{\Big(\frac{\epsilon}{\frac{\sigma}{\sqrt{n}}}\Big)^2} = \frac{\sigma^2}{n\epsilon^2}$$

which goes to zero as $n \to \infty$ for all $\epsilon > 0$, hence proving that $\bar{X}_n \xrightarrow{p} \mu$. □

The law of large numbers say that the event that $\bar{X}_n$ deviates from μ by more than ϵ become less and less probable as n increases. Hence, the distribution of $\bar{X}_n$ becomes more and more tightly concentrated around μ as n grows larger; regardless of how intolerant we are to deviations from μ, i.e. for all $\epsilon > 0$, we can always find a large enough sample size n so that the sample mean $\bar{X}_n$ is sufficiently close to μ. Figure 5.9 illustrates, and this observable widget provides a similar graph with interactivity.

The law of large numbers in Theorem 5.3 can be shown to hold more generally, also for certain dependent variables, and also without the assumption of a finite variance.

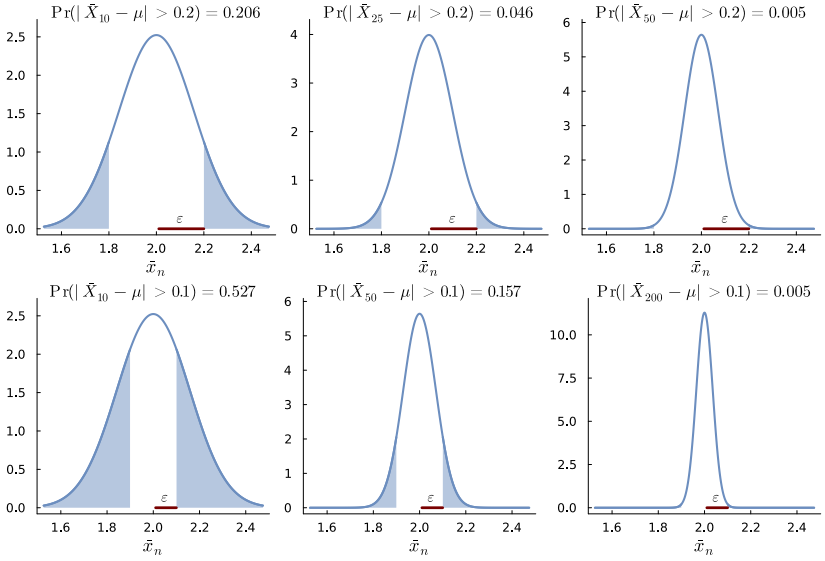

Figure 5.9: Illustration of the law of large numbers for a sample from a normal population $N(\mu = 2, \sigma^2 = 0.5^2)$. The shaded areas is the region where $|\bar{X}_n - \mu| \geq \varepsilon$. The top row uses a tolerance of $\epsilon = 0.2$ and the bottom row uses the harsher $\epsilon = 0.1$. The columns correspond to different sample sizes n as indicated by the subscript on $\bar{X}_n$ in the titles. Regardless of the tolerance ϵ we can choose n large enough to make the shaded region as small as we wish; note that the graphs in the second and third column uses different sample sizes n in the two rows.

5.4 *The central limit theorem*

In statistical inference, it is often important to know the distribution of the *sample mean*

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

of independent random variables $X_1, X_2, \ldots, X_n$. We again use a subscript n on $\bar{X}_n$ to explicitly show that the sample mean is based on n observations. This is useful here since we will now investigate how the distribution of the sample mean changes as n increases. We have seen in Chapter 4, that when the sample are independent draws from a normal distribution $X_1, X_2, \ldots, X_n \overset{\text{iid}}{\sim} N(\mu, \sigma^2)$, then the sample mean $\bar{X}_n$ is also normally distributed

$$\bar{X}_n \sim N\left(\mu, \frac{\sigma^2}{n}\right).$$

with a variance that decreases with n.

What can be said about the distribution of the sample mean when the data do *not* come from a normal distribution? In this section we will learn about the remarkable result that the distribution of the sample mean $\bar{X}_n$ approaches a certain distribution as n increases, *regardless of the distribution of the* $X_1, X_2, \ldots, X_n$. This is known as

the **central limit theorem** (CLT). The CLT may qualify as one of the seven wonders of the world, it is a wonderful result at the core of Statistics.

The law of large numbers tells us that the distribution of the sample mean $\bar{X}_n$ gets more and more concentrated around the population mean μ as n increases; $\bar{X}_n$ convergence in probability to μ as $n \to \infty$. However, it does not tell us anything about the *shape* of the distribution of $\bar{X}_n$ for large n, technically as $n \to \infty$. Studying this behavior of the distribution of $\bar{X}_n$ requires that we *normalize* the sample mean $\bar{X}_n$ in some way, because otherwise it will escape into a degenerate point mass at μ as $n \to \infty$, as dictated by the law of large numbers and illustrated in the graphs in the first row of Figure 5.10.

The natural way to normalize the sample mean is to standardize it:

$$\frac{\bar{X}_n - \mu}{\sigma/\sqrt{n}} = \frac{\sqrt{n}(\bar{X}_n - \mu)}{\sigma} \tag{5.4}$$

Note that the standardization is done by subtracting the expected value of the sample mean $\mathbb{E}(\bar{X}_n) = \mu$ and dividing by the standard deviation of the sample mean $\mathbb{S}(\bar{X}_n) = \sigma/\sqrt{n}$; these formulas were shown in Chapter 3 to be valid for the sample mean based on iid random variables from any distribution with finite mean and variance.

Figure 5.10 illustrates the effect of normalization for the case when $X_1, \ldots, X_n \overset{\text{iid}}{\sim} \text{Expon}(2)$. Each graph shows the distribution of the sample mean $\bar{X}_n$ obtained by simulating 10000 datasets with n observations and computing the sample mean for each of the 10000 datasets. The first row shows the distribution of the unnormalized sample mean $\bar{X}_n$ which collapses to a point mass at $\mu = 2$ as n increases; this is the law of large numbers in effect. The second row shows the distribution of the standardized sample mean which has a distribution that seems to settle down to a non-degenerate distribution as n increases. The final row shows the distribution of $n(\bar{X}_n - \mu)$; this is clearly not the correct normalization since the spread of the distribution is blowing up as n increases.

Figure 5.10 shows two more interesting things. First, the distribution of the standarized sample mean seems to settle down to a fixed distribution already after $n = 100$ observations, perhaps even earlier. This suggests that the asymptotic distribution of the sample mean as $n \to \infty$ may be a good approximation already for moderate sample sizes. Second, the distribution of the standarized sample mean seems to approach a standard *normal* distribution $N(0, 1)$ in large samples.

Figure 5.10 was based on data from the Expon(2) distribution. Figure 5.11 shows that this convergence of the (standardized) sample mean to a normal distribution holds for a number of other distributions. Again, the convergence is rather quick, and the distribution of

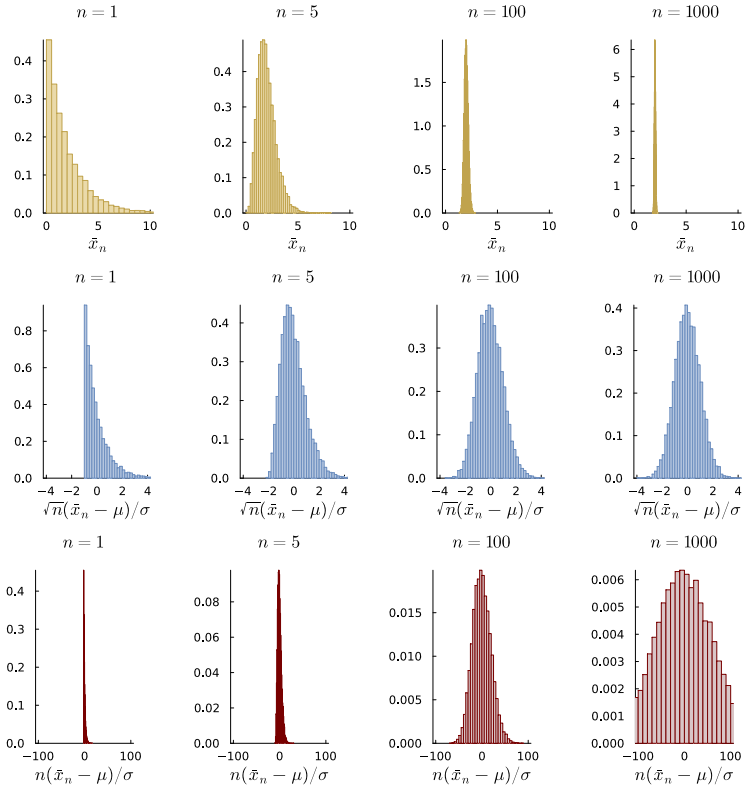

Figure 5.10: Illustrating the importance of proper normalization of the sample mean $\bar{X}_n$ in the central limit theorem with data sampled from the Expon(2) distribution. The top row shows that the distribution of the unnormalized sample mean $\bar{X}_n$ collapses to a degenerate point mass as the sample size increases. The second row shows that the distribution of $n(\bar{X}_n - \mu)$ is not using the correct normalization since the spread of the distribution is blowing up as n increases. The third row shows the distribution of the standardized sample mean $\frac{\bar{X}_n - \mu}{\sigma/\sqrt{n}} = \frac{\sqrt{n}(\bar{X}_n - \mu)}{\sigma}$, which has a distribution that seems to settle down to a non-degenerate distribution as n increases.

the standardized sample mean is already close to a normal distribution for $n = 100$ for all three distributions.

The next result shows that the above observations are not just coincidences, but that the distribution of the sample mean $\bar{X}_n$ converges to a normal distribution as $n \to \infty$ for *any* distribution of the $X_1, X_2, \ldots, X_n$ with finite mean and variance. The result is known as the **central limit theorem** (CLT).

central limit theorem

Theorem 8 (central limit theorem)**.**
Let $X_1, X_2, \ldots$ be iid random variables with finite mean μ and variance σ^2. Then

$$\frac{\bar{X}_n - \mu}{\sigma/\sqrt{n}} \xrightarrow{d} \mathrm{N}(0, 1),$$

as $n \to \infty$, where $\xrightarrow{d}$ denotes convergence in distribution.

How *fast* the distribution of the sample mean approaches a normal distribution depends on the distribution for the $X_1, X_2, \ldots, X_n$. For example, the distribution of the sample mean $\bar{X}_n$ from a normal distribution is already normal for all n, while the distribution of the sample mean $\bar{X}_n$ from the Chi-square distribution with $\nu = 1$ degrees

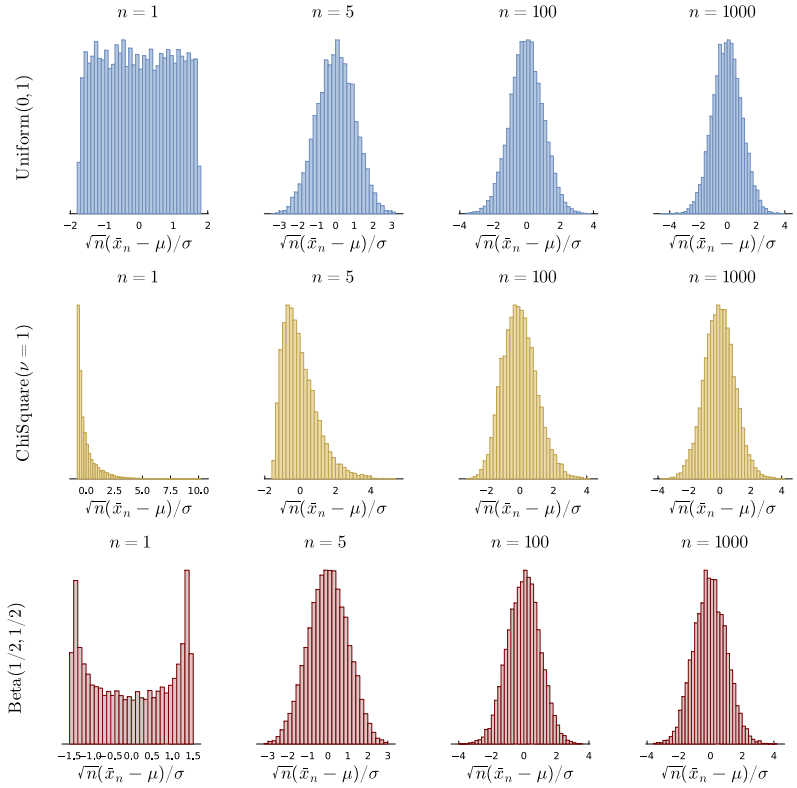

Figure 5.11: Illustrating of the central limit theorem by plotting simulated distributions for the sample mean for different sample sizes (columns) and for data from different distributions: Uniform$(0,1)$ (top row), Chi-squared with $\nu = 1$ degrees of freedom (middle row) and Beta$(1/2, 1/2)$ (bottom row).

of freedom needs a larger n than, for example, the Beta$(1/2, 1/2)$ distribution to approach a normal distribution. Nevertheless, the convergence is in general rather quick so the normal approximation suggested by the CLT is often used even for small sample sizes. A common rule of thumb in basic statistics course is that whenever $n \geq 30$, the normal approximation from the CLT is accurate. The normal approximation from the CLT is best expresses as the following *informal* version of the CLT.

Theorem 9 (central limit theorem - informal version)**.** *Let $X_1, X_2, \ldots$ be iid random variables with finite mean μ and variance σ^2. Then for large n,*

$$\bar{X}_n \overset{\text{approx}}{\sim} \mathrm{N}(\mu, \sigma^2/n)$$

This observable widget lets you explore the central limit theorem by exploring the distribution of the sample mean for different distributions and sample sizes.

The requirement of a finite mean and variance in the CLT are important. One example of a distribution for which the CLT does **not** hold is the Cauchy distribution introduced in Section 4.10. Fig-

ure 5.12 shows the failure of the CLT for the Cauchy distribution where the distribution for the sample mean (blue histogram) does not converge to a normal distribution as n increases. The tails of the histograms decay too slowly for it to be normal distribution; in fact, the histograms exclude the most extreme sample means for which $|\bar{x}_n| > 10$ for visualization purposes. Note that the sample mean is not standardized in the figure, since the mean and standard deviation do not exist; however, there seems to be no need for a normalization since the distribution for the unnormalized $\bar{X}_n$ actually does seem to settle down as $n \to \infty$. Even more, the distribution for the sample mean of Cauchy observations seems to be the *same distribution* for all n! That is indeed the case, and one can show that if $X_1, X_2, \ldots, X_n \overset{\text{iid}}{\sim} \text{Cauchy}(m, \tau^2)$ then

$$\bar{X}_n \sim \text{Cauchy}(m, \tau^2) \quad \text{for all } n.$$

So the sample mean of Cauchy observations is distributed as the *same* Cauchy distribution that generated the data $X_1, X_2, \ldots, X_n$; we say that the Cauchy distribution is **stable**. The heavy tails of the Cauchy distribution with occasional extreme values invalidates the averaging effect in the CLT.

stable

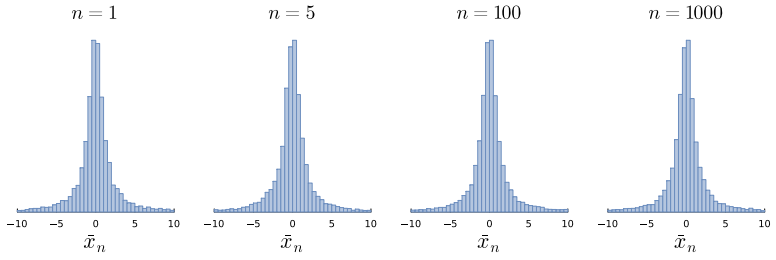

Figure 5.12: The figure shows the distribution of the sample mean $\bar{X}_n$ with iid data from the Cauchy distribution. The infinite mean and variance of the Cauchy distribution violates the conditions for the central limit theorem, and the sample mean does not converge in distribution to a normal distribution.

6 Transformation of random variables

In Chapters 3 and 4 we have learned about the most common univariate distributions and their properties. In this chapter we will learn how to derive the distribution for a function of a random variable, and how to use Monte Carlo simulation to generate random variables from any distribution, to compute expected values and tail probabilities.

6.1 Transformation of random variables

A common situation is that we have a random variable X with a known distribution, and we want to find the distribution of a transformed random variable $Y = g(X)$, where g is some function. In this section we will learn how to find the distribution of Y given the distribution of X. We have already seen some examples of distributions of transformed random variables:

- If $X \sim N(\mu, \sigma^2)$ and $Y = g(X)$ where $g(X) = a + bX$ is a linear transformation, then $Y = N(a + b\mu, b^2\sigma^2)$.
- If $X \sim N(0, 1)$ and $Y = g(X)$ where $g(X) = X^2$, then Y is a chi-squared random variable with 1 degree of freedom.
- If $X \sim \text{Gamma}(\alpha, \beta)$ and $Y = g(X)$ where $g(X) = c \cdot X$, for some constant $c > 0$ then $Y \sim \text{Gamma}(\alpha, c \cdot \beta)$.

All of these examples can be derived using the *transformation formula* given below; the name *change-of-variable formula* is more common, but less informative. We will work us up to the general result in three steps of increasing generality; we start with the case of a specific linear transformation, then move on to a slightly more general case with arbitrary intercept a and slope b in the linear transformation, and finally we will derive the change-of-variable formula for a general transformation $g(X)$.

Example: Let the random variable X have the pdf

$$f_X(x) = 3x^2, \text{ for } 0 \leq x \leq 1.$$

The upper left graph in Figure 6.1 shows the pdf. What is the cdf $F_Y(y)$ of the transformed variable $Y = 2 + 3X$? The cdf of Y is given by

$$F_Y(y) = \Pr(Y \leq y) = \Pr(2 + 3X \leq y) = \Pr\Big(X \leq \frac{y-2}{3}\Big) = F_X\Big(\frac{y-2}{3}\Big),$$

where $F_X(x)$ is the cdf of X. Note how we solved the inequality $2 + 3X \leq y$ in terms of X, to get X alone on the left hand side, so that we could use the definition of the cdf for X in the final step. This is clever since we know the pdf of X, and can therefore easily derive its cdf as

$$F_X(x) = \int_0^x f_X(t)dt = \int_0^x 3t^2 dt = [t^3]_0^x = x^3.$$

This cdf is displayed in the lower left graph in Figure 6.1. The cdf of Y can now be calculated from the cdf of X:

$$F_Y(y) = F_X\Big(\frac{y-2}{3}\Big) = \Big(\frac{y-2}{3}\Big)^3.$$

To find the pdf of Y, we take the first derivate of the cdf, using the chain rule:

$$f_Y(y) = \frac{\mathrm{d}}{\mathrm{d}y}F_Y(y) = \frac{\mathrm{d}}{\mathrm{d}y}\left(\frac{y-2}{3}\right)^3 = 3\Big(\frac{y-2}{3}\Big)^2 \cdot \frac{1}{3} = \Big(\frac{y-2}{3}\Big)^2.$$

Since the support of X is $0 \leq x \leq 1$, the support for the transformed variable is $2 \leq y \leq 5$. The pdf of Y is therefore

$$f_Y(y) = \frac{(y-2)^2}{9}, \text{ for } 2 \leq y \leq 5.$$

The pdf and cdf of Y are shown in the right column of Figure 6.1.

The next example is a direct repetition of the previous example, but now using a general linear transformation $Y = a + bX$, where a and b are arbitrary constants.

EXAMPLE: Let the random variable X have pdf

$$f_X(x) = 3x^2, \text{ for } 0 \leq x \leq 1.$$

What is the cdf $F_Y(y)$ of the transformed variable $Y = a + bX$? Consider first the case with a positive $b > 0$. The cdf of Y is given by

$$F_Y(y) = \Pr(Y \leq y) = \Pr(a + bX \leq y) = \Pr\Big(X \leq \frac{y-a}{b}\Big) = F_X\Big(\frac{y-a}{b}\Big),$$

where $F_X(x)$ is the cdf of X. Note that when solving for X in the inequality we implicitly used that $b > 0$; if $b < 0$, then the inequality sign has to be reversed, and we will deal with that case soon. The cdf of Y can again be expressed in terms of the cdf of X:

$$F_Y(y) = F_X\Big(\frac{y-a}{b}\Big) = \Big(\frac{y-a}{b}\Big)^3,$$

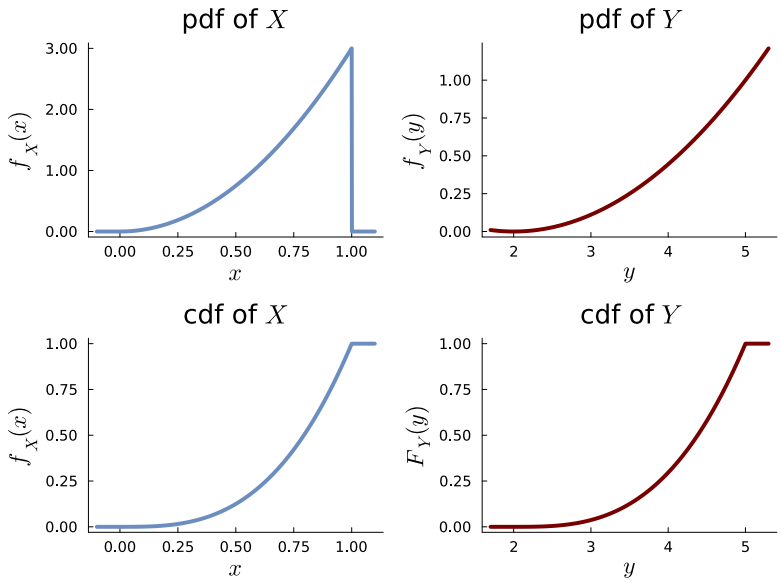

Figure 6.1: The transformation of the random variable X with pdf $f_X(x) = 3x^2$ for $0 \leq x \leq 1$ and cdf $F_X(x) = x^3$ (left column) to the random variable $Y = 2 + 3X$ (right column).

and the pdf of Y is given by

$$f_Y(y) = \frac{\mathrm{d}}{\mathrm{d}y} F_Y(y) = \frac{\mathrm{d}}{\mathrm{d}y} \left(\frac{y-a}{b} \right)^3 = 3 \Big(\frac{y-a}{b} \Big)^2 \cdot \frac{1}{b}.$$

Since the support of X is $0 \leq x \leq 1$, the support for the transformed variable is $a \leq y \leq a + b$. The pdf of Y is therefore

$$f_Y(y) = 3 \Big(\frac{y-a}{b} \Big)^2 \cdot \frac{1}{b}, \text{ for } a \leq y \leq a + b.$$

Let us now consider the case with a negative $b < 0$. The cdf of Y is given by

$$\begin{aligned} F_Y(y) &= \Pr(Y \leq y) = \Pr(a + bX \leq y) = \Pr\Big(X \geq \frac{y-a}{b} \Big) \\ &= 1 - \Pr\Big(X < \frac{y-a}{b} \Big) = 1 - F_X\Big(\frac{y-a}{b} \Big) \\ &= 1 - \Big(\frac{y-a}{b} \Big)^3. \end{aligned}$$

Note that the inequality sign is reversed when solving for X since we divide both sides of the inequality with the *negative* b; see Section 1.3 on inequalities. Finally, the pdf of Y is

$$f_Y(y) = \frac{\mathrm{d}}{\mathrm{d}y} F_Y(y) = -\frac{\mathrm{d}}{\mathrm{d}y} \left(\frac{y-a}{b} \right)^3 = -3 \Big(\frac{y-a}{b} \Big)^2 \cdot \frac{1}{b}.$$

Since $b < 0$, this last expression can be written with the absolute value $|\cdot|$ as

$$f_Y(y) = 3 \Big(\frac{y-a}{b} \Big)^2 \cdot \Big| \frac{1}{b} \Big|.$$

With this notation we can cover the two cases with positive and negative b in one expression. The pdf of $Y = a + bX$ for any constants a and b is therefore

$$f_Y(y) = 3\Big(\frac{y-a}{b}\Big)^2 \cdot \Big|\frac{1}{b}\Big|, \text{ for } a \leq y \leq a+b.$$

If we stare a little at the last expression, we can see a general rule. Solving the linear transformation $Y = a + bX$ for X gives $X = \frac{Y-a}{b}$, and this is by definition the *inverse function* $g^{-1}(Y) = \frac{Y-a}{b}$ of $g(X) = a + bX$; see Section 1.10. Hence, the first factor in (6.1) is

$$3\Big(\frac{y-a}{b}\Big)^2 = f_X\Big(g^{-1}(y)\Big).$$

This is the pdf of X evaluated at the inverse function $g^{-1}(y)$. Finally, the expression inside the absolute value in (6.1), $\frac{1}{b}$, is the derivative of the inverse function $g^{-1}(Y)$

$$\frac{\mathrm{d}}{\mathrm{d}y}g^{-1}(y) = \frac{\mathrm{d}}{\mathrm{d}y}\left(\frac{y-a}{b}\right) = \frac{1}{b}.$$

After all this work, it should be easier to follow the following derivation of the general change-of-variable formula for a transformed random variable $Y = g(X)$, where g is an monotonically increasing function with continuous derivative. Here we go:

$$F_Y(y) = \Pr(Y \leq y) = \Pr(g(X) \leq y) = \Pr\Big(X \leq g^{-1}(y)\Big) = F_X\Big(g^{-1}(y)\Big).$$

Note that we implicitly applied the inverse function $g^{-1}(y)$ to both sides of the inequality $g(X) \leq y$ to solve for X on the left hand side:

$$g(X) \leq y \iff g^{-1}(g(X)) \leq g^{-1}(y) \iff X \leq g^{-1}(y).$$

since $g^{-1}(g(X)) = X$ by the definition of an inverse function; also, the inequality sign is not reversed since g is a monotonically increasing function. The pdf of Y is then easily obtained with the chain rule as

$$f_Y(y) = \frac{\mathrm{d}}{\mathrm{d}y}F_Y(y) = f_X\Big(g^{-1}(y)\Big) \cdot \frac{\mathrm{d}}{\mathrm{d}y}g^{-1}(y).$$

If the transformation is monotonically decreasing, we can use the same reasoning, but we have to remember that the inequality sign has to be reversed and the derivative of the inverse function is negative. Using the absolute value, as above, we can cover both cases with monotonically increasing or monotonically decreasing transformation $Y = g(X)$ in one formula. We summarize this result in Figure 6.1.

Distribution of a monotonic transformation of a random variable

Let $X \sim f_X(x)$ and let

$$Y = g(X)$$

be a monotone transformation with an inverse transformation

$$X = g^{-1}(Y)$$

with a continuous derivative. The density of Y is then

$$f_Y(y) = f_X\Big(g^{-1}(y)\Big) \left| \frac{\mathrm{d}}{\mathrm{d}y} g^{-1}(y) \right|$$

Figure 6.2: The transformation formula to calculate the density of a monotonic function of a random variable.

EXAMPLE: Let $X \sim N(\mu, \sigma^2)$ with pdf

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}, \text{ for } -\infty < x < \infty.$$

What is the pdf of the transformed variable $Y = \exp(X)$? This is a monotonically increasing function and we can apply the result in Figure . The inverse function of the exponential function is the natural logarithm function $g^{-1}(y) = \log(y)$, and its derivative is

$$\frac{\mathrm{d}}{\mathrm{d}y} g^{-1}(y) = \frac{1}{y}.$$

The pdf of Y is then

$$\begin{aligned} f_Y(y) &= f_X\Big(g^{-1}(y)\Big) \left| \frac{\mathrm{d}}{\mathrm{d}y} g^{-1}(y) \right| \\ &= f_X\Big(\log(y)\Big) \cdot \frac{1}{y} = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(\log(y)-\mu)^2}{2\sigma^2}} \cdot \frac{1}{y}. \end{aligned}$$

The support of Y is $0 < y < \infty$. The distribution of $Y = \exp(X)$ when $X \sim N(\mu, \sigma^2)$ is the *LogNormal distribution* presented in Section 4.8. Figure 6.3 illustrates.

EXAMPLE: Let $X \sim \text{Gamma}(\alpha, \beta)$ with pdf

$$f_X(x) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x}, \text{ for } 0 < x < \infty.$$

What is the pdf of the scaled variable $Y = cX$, for some positive constant $c > 0$? The inverse function is $g^{-1}(y) = \frac{y}{c}$, with derivative

$$\frac{\mathrm{d}}{\mathrm{d}y} g^{-1}(y) = \frac{1}{c}.$$

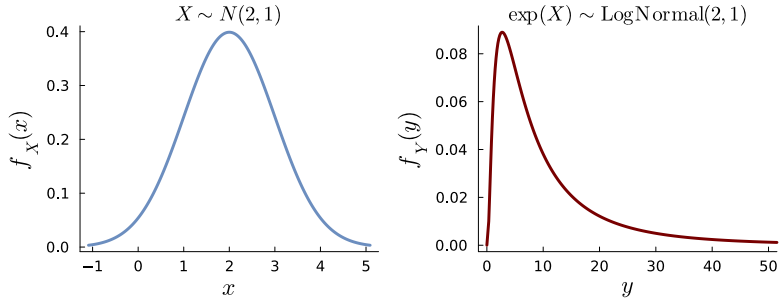

Figure 6.3: LogNormal distribution is the exponential transformation of a normal random variable.

Since the pdf of $X \sim \text{Gamma}(\alpha, \beta)$ is

$$f_X(x) = \frac{1}{\beta^\alpha \Gamma(\alpha)} x^{\alpha-1} e^{-\frac{x}{\beta}}, \text{ for } 0 < x < \infty,$$

the pdf of $Y = cX$ is

$$f_Y(y) = f_X\Big(g^{-1}(y)\Big) \left| \frac{\mathrm{d}}{\mathrm{d}y} g^{-1}(y) \right| \tag{6.1}$$

$$= f_X\Big(\frac{y}{c}\Big) \cdot \frac{1}{c} = \frac{1}{\beta^\alpha \Gamma(\alpha)} \Big(\frac{y}{c}\Big)^{\alpha-1} e^{-\frac{y}{c\beta}} \cdot \frac{1}{c} \tag{6.2}$$

$$= \frac{1}{(c\beta)^\alpha \Gamma(\alpha)} y^{\alpha-1} e^{-\frac{y}{c\beta}}. \tag{6.3}$$

The support of Y is $0 < y < \infty$. This density of $Y = cX$ in (6.1) is again a *gamma distribution*, but where the scale parameter β has been replaced by $c\beta$. We say that the gamma distribution is a *closed under positive scaling* since multiplication of a Gamma variable with positive constant c gives another gamma variable with the same shape parameter α and a new scale parameter $c\beta$. We can summarize this as

$$\text{If } X \sim \text{Gamma}(\alpha, \beta) \text{ then } cX \sim \text{Gamma}(\alpha, c\beta).$$

EXAMPLE: If $X \sim \chi^2(\nu)$, then the distribution of $Y = \nu\tau^2 \frac{1}{X}$ is called the **scaled inverse chi-squared distribution** with scale parameter σ^2 and ν degrees of freedom. As the name suggests, it is the distribution of the inverse of a χ^2 variable scaled by a positive constant. The distribution plays an important role in Bayesian learning. Using the transformation formula, we can derive the pdf of Y as follows. The inverse function is $g^{-1}(y) = \frac{\nu\tau^2}{y}$, with derivative

scaled inverse chi-squared distribution

$$\frac{\mathrm{d}}{\mathrm{d}y} g^{-1}(y) = -\frac{\nu\tau^2}{y^2}.$$

The pdf of $X \sim \chi^2(\nu)$ is

$$f_X(x) = \frac{1}{2^{\nu/2}\Gamma(\nu/2)} x^{\nu/2-1} e^{-\frac{x}{2}}, \text{ for } 0 < x < \infty,$$

and the pdf of $Y = \nu\tau^2 \frac{1}{X}$ is

$$\begin{aligned} f_Y(y) &= f_X\Big(g^{-1}(y)\Big) \left| \frac{\mathrm{d}}{\mathrm{d}y} g^{-1}(y) \right| \\ &= f_X\Big(\frac{\nu\tau^2}{y}\Big) \cdot \Big(\frac{\nu\tau^2}{y^2}\Big) \\ &= \frac{1}{2^{\nu/2}\Gamma(\nu/2)} \Big(\frac{\nu\tau^2}{y}\Big)^{\nu/2-1} e^{-\frac{\nu\tau^2}{2y}} \cdot \Big(\frac{\nu\tau^2}{y^2}\Big) \\ &= \frac{1}{2^{\nu/2}\Gamma(\nu/2)} \cdot \frac{(\nu\tau^2)^{\nu/2}}{y^{\nu/2+1}} \cdot e^{-\frac{\nu\tau^2}{2y}} \\ &= \frac{(\nu\tau^2/2)^{\nu/2}}{\Gamma(\nu/2)} \cdot \frac{e^{-\frac{\nu\tau^2}{2y}}}{y^{\nu/2+1}}, \end{aligned}$$

with support $0 < y < \infty$. The scaled inverse chi-squared distribution is denoted by Inv-$\chi^2(\nu, \tau^2)$ or the little longer Scaled-Inv-$\chi^2(\nu, \tau^2)$. Figure 6.4 plots the pdf of a χ^2 variable with $\nu = 3$ degrees of freedom (blue) and some scaled inverse chi-squared distributions with $\nu = 3$ degrees of freedom and varying scale parameter τ^2.

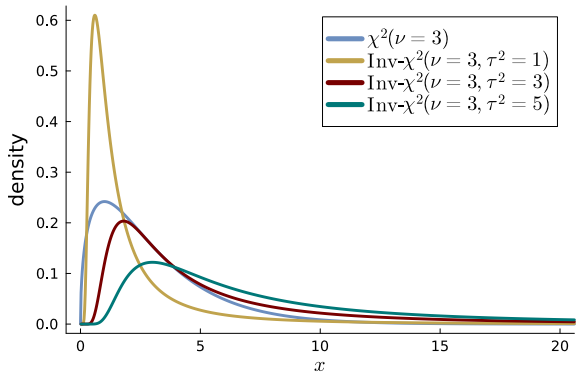

Figure 6.4: Illustration of how a scaled inverse chi-squared distributed variable, $Y \sim$ Inv-$\chi^2(\nu, \tau^2)$, is an inverted and scaled $\chi^2(\nu)$ variable.

If the transformation is not monotone over the whole domain of X, then it is usually monotone over subregions. Let $\mathcal{X}_j$ for $j = 1, \ldots, J$ be a partition of the domain $\mathcal{X}$ of X, i.e. a collection of disjoint intervals that together cover all of $\mathcal{X}$. Figure 6.5 gives the generalization of the transformation formula to the case where the transformation is monotone on each subinterval $\mathcal{X}_j$.

Distribution of a piecewise monotonic transformation of a random variable

Let $X \sim f_X(x)$ and

$$Y = g(X)$$

be a transformation that is monotone on each subinterval $\mathcal{X}_j$ of a partition of the domain of X and has the inverse transformation

$$X = g_j^{-1}(Y)$$

over $\mathcal{X}_j$, with a continuous derivative. The density of Y is then

$$f_Y(y) = \sum_{j=1}^{J} f_X\left(g_j^{-1}(y)\right) \left| \frac{\mathrm{d}}{\mathrm{d}y} g_j^{-1}(y) \right|$$

Figure 6.5: The transformation formula to calculate the density of a piecewise monontonic transformation with continuous derivatives on each subinterval.

EXAMPLE: Let $X \sim N(0,1)$ and consider the distribution of the square $Y = X^2$. This transformation is not monotone; for example, both $X = 1$ and $X = -1$ give the same value $Y = 1$. The transformation $Y = X^2$ is monotonically decreasing for $x \in (-\infty, 0]$ and monotonically increasing for $x \in (0, \infty)$; see Figure 6.6. Hence we use the transformation formula in Figure 6.5 with the partition $\mathcal{X} = (-\infty, 0] \cup (0, \infty)$. In the first interval $x \in (0, \infty)$, the inverse transformation is obtained by solving $y = x^2$ for x, with solution $x = \sqrt{y}$, and derivative

$$\frac{\mathrm{d}}{\mathrm{d}y} g^{-1}(y) = \frac{\mathrm{d}}{\mathrm{d}y} \sqrt{y} = -\frac{1}{2\sqrt{y}}.$$

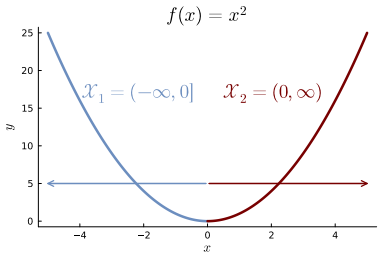

Figure 6.6: The transformation $Y = g(X)$ is piecewise monotone with two subintervals $\mathcal{X}_1 = (-\infty, 0]$ and $\mathcal{X}_2 = (0, \infty)$.

We therefore have for the subinterval $(0, \infty)$

$$\begin{aligned} f_X\left(g_1^{-1}(y)\right) \left| \frac{\mathrm{d}}{\mathrm{d}y} g_1^{-1}(y) \right| &= f_X\left(\sqrt{y}\right) \cdot \frac{1}{2\sqrt{y}} \\ &= \frac{1}{\sqrt{2\pi}} e^{-\frac{(\sqrt{y})^2}{2}} \cdot \frac{1}{2\sqrt{y}} = \frac{1}{2\sqrt{2\pi}} e^{-\frac{y}{2}} \cdot \frac{1}{\sqrt{y}} \\ &= \frac{1}{2 \cdot 2^{1/2} \mathrm{Gamma}(1/2)} y^{1/2-1} e^{-\frac{y}{2}}, \end{aligned} \tag{6.4}$$

where we have used that $\sqrt{\pi} = \mathrm{Gamma}(1/2)$ and the other seemingly meaningless manipulations have been done to get the density in the form that the chi-squared distribution is usually presented in. The derivation can be done for the subinterval $x \in (-\infty, 0)$ to obtain exactly the same expression as in (6.4). From Figure 6.5, the density

of Y is therefore given by the sum of the contributions from the two subintervals:

$$\begin{aligned} f_Y(y) &= f_X\left(g_1^{-1}(y)\right)\left|\frac{\mathrm{d}}{\mathrm{d}y}g_1^{-1}(y)\right| + f_X\left(g_2^{-1}(y)\right)\left|\frac{\mathrm{d}}{\mathrm{d}y}g_2^{-1}(y)\right| \\ &= \frac{1}{2^{1/2}\text{Gamma}(1/2)}y^{1/2-1}e^{-\frac{y}{2}}, \end{aligned}$$

which is the density of a χ^2 variable with $\nu = 1$ degree of freedom.

We end this section with an important transformation result when the cdf itself is used as the transformation function. The **probability integral transform** states that if X is a continuous random variable with cdf $F_X(x)$, then the random variable $Y = F_X(X)$ is uniformly distributed on the interval $(0, 1)$. As we will see in the next section, this result allows us to generate random variables from any distribution by first generating a uniform random variable and then applying the inverse cdf of the desired distribution. Figure 6.7 illustrates the probability integral transform. The top row shows 10 draws, plotted as yellow dots on the horizontal axis, from the exponential distribution with $\beta = 1$ (left) and the beta distribution (right). The cdf value $Y = F_X(x)$ for each draw is displayed as a red dot on the vertical axis. The bottom row plots histogram based on 10000 cdf values $Y_i = F_X(X_i)$, where X_i are random draws from the exponential distribution (left) and the beta distribution (right). The histogram of the cdf values are close to the uniform distribution on $(0, 1)$, as expected by the probability integral transform.

probability integral transform

Theorem 10. *Let X be a continuous random variable with cdf $F_X(x)$. Then,*

$$Y = F_X(X) \sim \mathrm{U}(0, 1)$$

Proof. Assume that $F_X(x)$ is a continuous and strictly increasing function. The cdf of Y is given by

$$\begin{aligned} F_Y(y) &= \Pr(Y \leq y) = \Pr(F_X(X) \leq y) \\ &= \Pr(X \leq F_X^{-1}(y)) = F_X(F_X^{-1}(y)) = y, \end{aligned}$$

where we have used that $F_X(x)$ is a monotonically increasing function and therefore has an inverse such that $F_X(F_X^{-1}(y)) = y$ for all $y \in (0, 1)$. The cdf of Y is therefore $F_Y(y) = y$ for $0 < y < 1$, which is the cdf of a uniform distribution on $(0, 1)$. The proof for the case with $F_X(x)$ not being strictly increasing is similar, but we have to be careful with the inverse function, see Casella and Berger (2002) for details. □

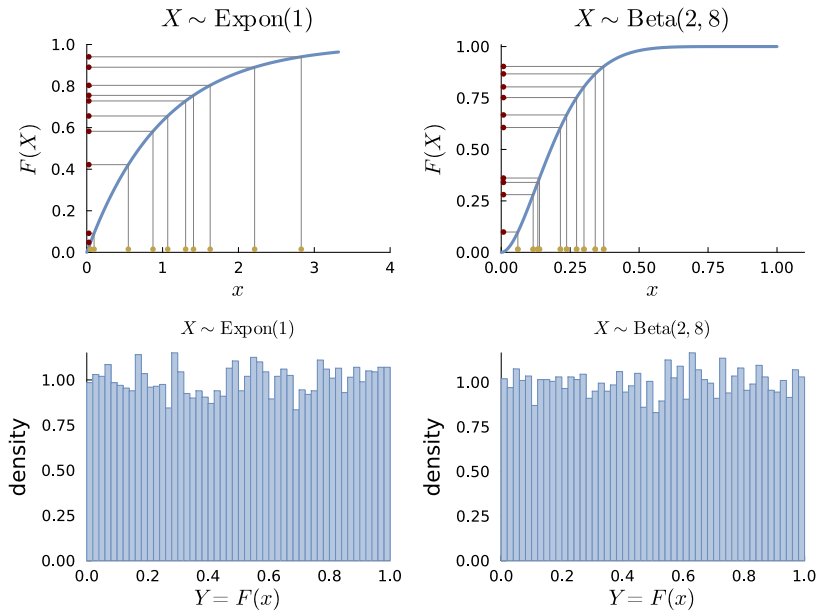

Figure 6.7: Illustration of the probability integral transform. The cdf values $Y_i = F_X(X_i)$ (red dots) for 10 random draws $X_i \overset{\text{iid}}{\sim} F_X(x)$ (yellow dots) follow a uniform distribution on $[0, 1]$.

EXERCISES

Transformation of random variables

1. Let X have density
$$f_X(x) = \frac{x}{2}$$
for $0 < x < 2$. Derive the cdf $F_Y(y)$ and pdf $f_Y(y)$ of the transformed variable $Y = \exp(X)$.
2. Let $X \sim \text{Uniform}(0, 1)$ follow uniform distribution over $0 \leq x \leq 1$. What is the density of $Y = -\beta \log(X)$, where β is a positive constant? Do you recognize this distribution as one of the distributions presented in the book?
3. Let $X \sim \text{Beta}(\alpha, \beta)$. Determine the density of the so called log-odds:
$$Y = \log\left(\frac{X}{1 - X}\right)$$

6.2 *Monte Carlo simulation*

7 Joint distributions

7.1 Joint, marginal and conditional distributions for discrete random variables

Joint distribution for discrete random variables

In the Chapter Probability we defined the simultaneous probability of two events A and B as the probability that both events occur

$$\Pr(A \cap B) = \Pr(A \text{ and } B), \tag{7.1}$$

where $A \cap B$ is the intersection of the two events. The **joint probability function** for two discrete random variables X and Y is a bivariate function that returns the probability of the event that $X = x$ *and* $Y = y$, for some pair of values x and y.

joint probability function

Definition. *The joint probability function for two discrete random variables X and Y is given by*

$$p(x, y) = \Pr(X = x, Y = y) \tag{7.2}$$

The joint probability function is often called the *joint probability distribution*, or simply the **joint distribution**, or the little more cumbersome **joint probability mass function**.

joint distribution

joint probability mass function

A joint probability function for two discrete random variables X and Y satisfies the following properties:

- $0 \leq p(x, y) \leq 1$ for all x, y
- $\sum_x \sum_y p(x, y) = 1$

where the sums are over all possible values of x and y.

Example: Consider again the experiment of rolling two dice, but this time letting one random variable X count the number of dice with 5 dots and another random variable Y counting the sum of dots on the two dice. The joint distribution of X and Y is given in Table

7.1 and visualized in Figure 7.1. For example, the probability of a sum of $Y = 7$ dots, with exactly one die with 5 dots ($X = 1$) is $\frac{2}{36}$; as there are only two outcomes out of 36 possible outcomes that satisfy $X = 1$ and $Y = 7$: namely the outcomes: $(5, 2)$ and $(2, 5)$. The outcome $X = 1$ and $Y = 10$ has probability zero since the only outcomes with a sum of $Y = 10$ dots is $(4, 6), (6, 4), (5, 5)$, and none of these outcomes satisfy the condition of having *exactly one* die with 5 dots ($X = 1$).

$X \backslash Y$	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
0	$\frac{1}{36}$	$\frac{2}{36}$	$\frac{3}{36}$	$\frac{4}{36}$	$\frac{3}{36}$	$\frac{4}{36}$	$\frac{3}{36}$	$\frac{2}{36}$	$\frac{2}{36}$	$\frac{0}{36}$	$\frac{1}{36}$
1	0	0	0	0	$\frac{2}{36}$	$\frac{2}{36}$	$\frac{2}{36}$	$\frac{2}{36}$	0	$\frac{2}{36}$	0
2	0	0	0	0	0	0	0	0	$\frac{1}{36}$	0	0

Table 7.1: Joint probability distribution $p(x, y)$ of the number of dice with 5 dots ($X =$) and the sum of dots on two dice (Y) when rolling two dice.

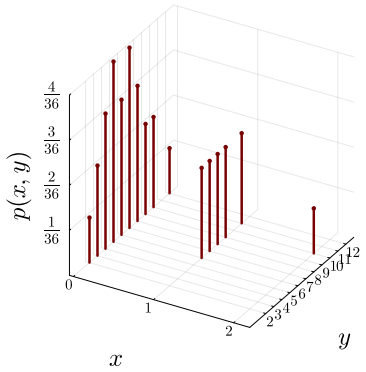

Figure 7.1: Joint probability distribution $p(x, y)$ of the number of dice with 5 dots (X) and the sum of dots on two dice (Y) when rolling two dice.

Marginal distributions for discrete random variables

The *marginal distribution* of X is the probability distribution for all values for X *regardless of what happens to* Y. This means that the probability for a specific outcome $X = x$ is given by the sum of the joint probabilities $p(x, y)$ over all possible values of Y, as in the following definition.

Definition. *The marginal distribution for X is given by*

$$p_X(x) = \sum_y p(x, y) \tag{7.3}$$

where the sum is over all possible y values.

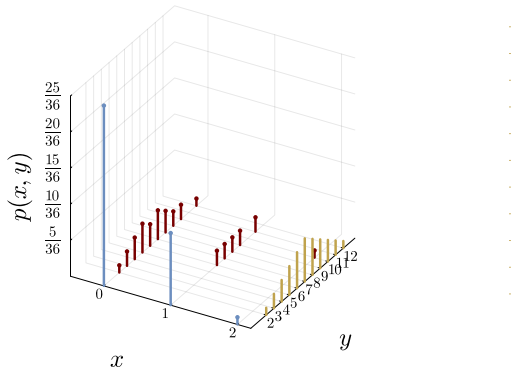

Figure 7.2: Joint $p(x,y)$ (red) and marginal probability distributions $p_X(x)$ (blue) and $p_Y(y)$ (yellow) of the number of dice with 5 dots (X) and the sum of dots on two dice (Y) when rolling two dice.

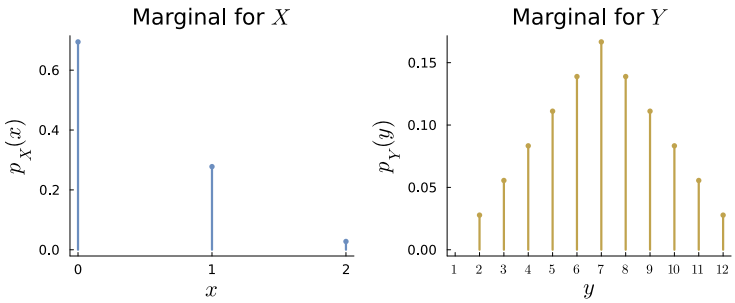

Figure 7.3: Rolling two dice. Marginal probability distributions for X = number of dice with 5 dots (left) and Y = sum of dots on two dice (right).

The marginal distribution for Y is defined in exactly the same way, but now summing over all possible values of X:

$$p_Y(y) = \sum_x p(x,y).$$

EXAMPLE: Rolling two dice. The marginal probability of $X = 0$, no dice with 5 dots, is obtained by summing all the joint probabilities on the first row in Table 7.1. The marginal probability for $x = 1$ and $x = 2$ is obtained by summing the second and third row, respectively. This gives the marginal distribution for X as

$$p_X(x) = \sum_y p(x,y) = \begin{cases} \frac{25}{36} & \text{for } x = 0 \\ \frac{10}{36} & \text{for } x = 1 \\ \frac{1}{36} & \text{for } x = 2 \end{cases} \tag{7.4}$$

Figure 7.2 replicates the previous table with the joint distribution, but adds the marginal distribution $p_X(x)$ for X in the last column. Similarly, the marginal distribition for Y is added as new row at the end of the table. The marginal probabilities for Y are obtained by summing each column. The marginal distribution for X is shown as the blue bars in Figure 7.2 and also in the left graph of Figure 7.3. The marginal distribution for Y, the sum of dots on two dice, is

shown as the yellow bars in Figure 7.2 and also in the right graph of Figure 7.3.

$X\backslash Y$	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	$p(x)$
0	$\frac{1}{36}$	$\frac{2}{36}$	$\frac{3}{36}$	$\frac{4}{36}$	$\frac{3}{36}$	$\frac{4}{36}$	$\frac{3}{36}$	$\frac{2}{36}$	$\frac{2}{36}$	0	$\frac{1}{36}$	$\frac{25}{36}$
1	0	0	0	0	$\frac{2}{36}$	$\frac{2}{36}$	$\frac{2}{36}$	$\frac{2}{36}$	0	$\frac{2}{36}$	0	$\frac{10}{36}$
2	0	0	0	0	0	0	0	0	$\frac{1}{36}$	0	0	$\frac{1}{36}$
$p(y)$	$\frac{1}{36}$	$\frac{2}{36}$	$\frac{3}{36}$	$\frac{4}{36}$	$\frac{5}{36}$	$\frac{6}{36}$	$\frac{5}{36}$	$\frac{4}{36}$	$\frac{3}{36}$	$\frac{2}{36}$	$\frac{1}{36}$	

Table 7.2: Joint probability distribution $p(x,y))$ of the number of dice with 5 dots (X) and the sum of dots on two dice (Y) when rolling two dice. The marginal distributions, written as $p(x)$ and $p(y)$ for brevity, are shown in the last column and last row, respectively.

Conditional distributions for discrete random variables

In the Chapter Probability we defined the conditional probability of an event A given the event B as the probability that A occurs given that B has occurred. The conditional probability is given by

$$\Pr(A|B) = \frac{\Pr(A \cap B)}{\Pr(B)} \tag{7.5}$$

assuming that B can occur, i.e. that $\Pr(B) > 0$.

We can similarly define the conditional distribution of a random variable Y given that some other variable X takes on a specific value x. The conditional distribution of Y given the outcome $X = x$ is the ratio of the joint distribution $p(x,y)$ to the marginal distribution $p_X(x)$. Here is the definition of a **conditional distribution**.

conditional distribution

Definition. *The conditional distribution of a discrete random variable Y given the outcome $X = x$ on some other discrete random variable is given by*

$$p_{Y|X}(y|x) = \frac{p(x,y)}{p_X(x)}$$

provided that $p_X(x) > 0$.

The conditional distribution of X given $Y = y$ is analogously given by

$$p_{X|Y}(x|y) = \frac{p(x,y)}{p_Y(y)}$$

provided that $p_Y(y) > 0$.

EXAMPLE: Rolling two dice. What is the conditional distribution for X, the number of fives, conditional on the sum of the two dice being

$y = 10$? We can use Table 7.2 to calculate the conditional probability $p_{X|Y}(x|y = 10)$ as follows:

$$p_{X|Y}(x = 0|y = 10) = \frac{p(x = 0, y = 10)}{p_Y(y = 10)} = \frac{\frac{2}{36}}{\frac{3}{36}} = \frac{2}{3}$$

since $p_Y(y = 10) = \frac{3}{36}$ is the marginal probability of $Y = 10$. Similarly for $x = 1$ and $x = 2$ we have

$$p_{X|Y}(x = 1|y = 10) = \frac{p(x = 1, y = 10)}{p_Y(y = 10)} = \frac{0}{\frac{3}{36}} = 0$$

and

$$p_{X|Y}(x = 2|y = 10) = \frac{p(x = 2, y = 10)}{p_Y(y = 10)} = \frac{\frac{1}{36}}{\frac{3}{36}} = \frac{1}{3}$$

Note that since a conditional distribution is a probability distribution, the conditional probabilities must sum to 1; we could therefore have calculated the last conditional probability from the other two by

$$\begin{aligned} p_{X|Y}(x = 2|y = 10) &= 1 - p_{X|Y}(x = 0|y = 10) - p_{X|Y}(x = 1|y = 10) \\ &= 1 - \frac{2}{3} - 0 = \frac{1}{3}. \end{aligned}$$

The conditional distribution of X given that the sum of the two dice is $Y = 10$ is shown in Figure 7.4 as the red bars. The marginal distribution of X is shown as the blue bars. It is clear that the knowledge of the sum of the two dice $Y = 10$ has changed the distribution of X from the marginal distribution. Once we know that the sum is ten, there is a substantial probability of two fives, an event that is rather unlikely in the marginal distribution.

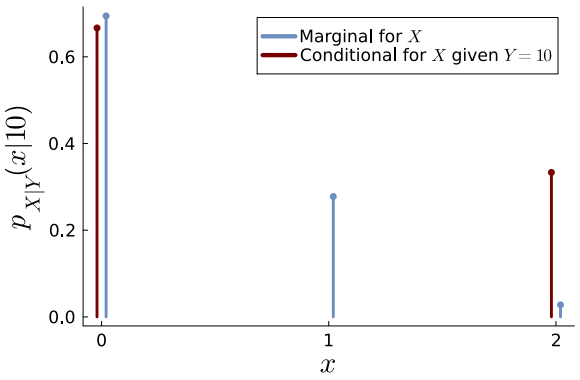

Figure 7.4: Rolling two dice. Conditional distribution of X = number of fives given that the sum of dice is $Y = 10$ (red bars). The marginal marginal distribution of X (blue bars) is given as reference.

7.2 *Joint, marginal and conditional distributions for continuous random variables*

Joint distribution for continuous variables

joint cumulative distribution function

The **joint cumulative distribution function** (joint cdf) for two random variables X and Y is given by

$$F(x, y) = \Pr(X \leq x, Y \leq y) \tag{7.6}$$

The joint cdf is the probability that X is less than or equal to x *and* that Y is less than or equal to y. This definition applies to both discrete and continuous random variables. Figure 7.5 illustrates a joint cumulative distribution function for two continuous random variables X and Y. The left graph plots the joint cdf as a surface while the right graph plots *level contours* of the joint cdf, where all (x, y) points on a given contour has the same joint probability. The blue color scale visualize the average probability between any two contour lines. The (x, y) points on a given contour has the same joint cdf $f(x, y)$.

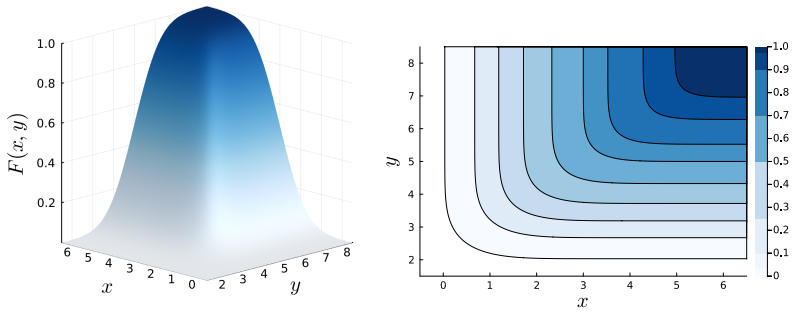

Figure 7.5: A joint cumulative distribution function (cdf) $F(x, y)$ for two continuous random variables X and Y. The left graph plots the joint cdf as a surface while the right graph plots level contours of the joint cdf, where all (x, y) points on a given contour has the same joint probability.

For a univariate continuous random variable X with cumulative distribution function (cdf) $F(x)$ we saw earlier that the probability density function (pdf) was the derivative of the cdf $f(x) = F'(x)$, and that probabilities could be computed by integrating under the pdf: $\Pr(a \leq X \leq b) = \int_a^b f(x)\,\mathrm{d}x$. We can similarly define the **joint probability density function** for two continuous random variables X and Y as the cross partial derivative of the joint cdf:

joint probability density function

$$f(x, y) = \frac{\partial^2 F(x, y)}{\partial x \partial y}, \tag{7.7}$$

where $F(x, y)$ is the joint cumulative distribution function (cdf) for X and Y. A joint pdf must satisfy

- $f(x, y) \geq 0$ for all x, y
- $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y)\,\mathrm{d}y\,\mathrm{d}x = 1$

- $\Pr(a \leq X \leq b, c \leq Y \leq d) = \int_a^b \int_c^d f(x,y)\,\mathrm{d}y\,\mathrm{d}x$

Figure 7.6 illustrates a joint probability density function for two continuous random variables, X and Y. The left graph plots the joint pdf as a surface and the right graph plots *level contours* of the joint pdf as black lines (ellipses in this case) with blue color scale visualize the average density between any two contour lines. The (x,y) points on a given contour has the same joint density $f(x,y)$.

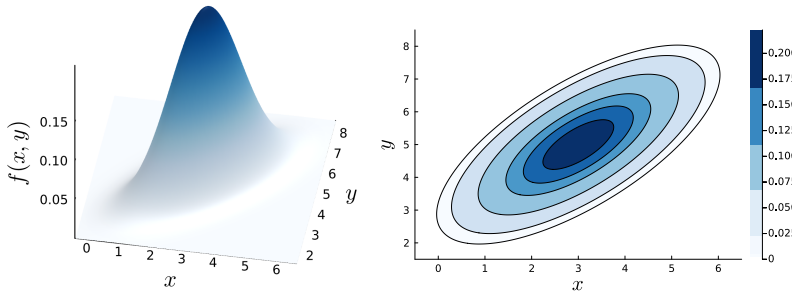

Figure 7.6: The joint probability density function (pdf) for two continuous random variables X and Y. The left graph plots the joint pdf as a surface while the right graph plots level contours of the joint pdf, where all (x,y) points on a given contour has the same joint density.

EXAMPLE: Consider the joint pdf for two continuous random variables X and Y given by

$$f(x,y) = \begin{cases} 6x^2y & \text{for } 0 < x < 1, 0 < y < 1 \\ 0 & \text{otherwise} \end{cases} \tag{7.8}$$

For this to be a joint density it must integrate to 1 over the entire (x,y)-space:

$$\begin{aligned} \int_0^1 \int_0^1 6x^2y\,\mathrm{d}y\,\mathrm{d}x &= \int_0^1 6x^2 \left(\int_0^1 y\,\mathrm{d}y \right) \mathrm{d}x = \int_0^1 6x^2 \left[\frac{y^2}{2} \right]_0^1 \mathrm{d}x \\ &= \int_0^1 6x^2 \cdot \frac{1}{2}\,\mathrm{d}x = 3\int_0^1 x^2\,\mathrm{d}x \\ &= 3\left[\frac{x^3}{3} \right]_0^1 = 3 \cdot \frac{1}{3} = 1, \end{aligned}$$

so this is indeed a joint pdf.

EXAMPLE: Consider the joint pdf for two continuous random variables X and Y given by

$$f(x,y) = \begin{cases} \frac{1}{x} e^{-\left(\frac{y}{x} + x\right)} & \text{for } 0 < x < \infty, 0 < y < \infty \\ 0 & \text{otherwise} \end{cases} \tag{7.9}$$

We can verify that this is a joint pdf by checking that it integrates to 1

over the entire (x, y)-space. Let us check this

$$\begin{aligned}\int_0^\infty \int_0^\infty \frac{1}{x} e^{-\left(\frac{y}{x}+x\right)}\, \mathrm{d}y\, \mathrm{d}x &= \int_0^\infty \frac{1}{x} e^{-x} \left(\int_0^\infty e^{-\frac{y}{x}}\, \mathrm{d}y \right) \mathrm{d}x \\ &= \int_0^\infty \frac{1}{x} e^{-x} \left[-x e^{-\frac{y}{x}} \right]_0^\infty \mathrm{d}x \\ &= \int_0^\infty \frac{1}{x} e^{-x} x\, \mathrm{d}x \\ &= \int_0^\infty e^{-x}\, \mathrm{d}x \\ &= [-e^{-x}]_0^\infty = 1.\end{aligned}$$

Marginal distributions for continuous variables

The marginal density for X is the same idea as in the case with discrete random variables, but instead of summing with respect to y we integrate the joint pdf with respect to y:

$$f_X(x) = \int f(x, y)\, \mathrm{d}y \tag{7.10}$$

The marginal density for Y is analogously given by

$$f_Y(y) = \int f(x, y)\, \mathrm{d}x \tag{7.11}$$

EXAMPLE: We revisit the joint pdf $f(x, y) = 6x^2 y$ for $0 < x < 1, 0 < y < 1$. The marginal pdf for X is obtained by integrating out y from the joint pdf:

$$f_X(x) = \int_0^1 6x^2 y\, \mathrm{d}y = 6x^2 \left[\frac{y^2}{2} \right]_0^1 = 3x^2, \quad 0 < x < 1$$

and $f_X(x) = 0$ otherwise. The marginal pdf for Y is obtained by integrating out x:

$$f_Y(y) = \int_0^1 6x^2 y\, \mathrm{d}x = 6y \left[\frac{x^3}{3} \right]_0^1 = 2y, \quad 0 < y < 1$$

and $f_Y(y) = 0$ otherwise.

EXAMPLE: Revisit the joint pdf for two continuous random variables X and Y given previously by

$$f(x, y) = \frac{1}{x} e^{-\left(\frac{y}{x}+x\right)}$$

for $0 < x < \infty, 0 < y < \infty$ and $f(x, y) = 0$ otherwise. The marginal pdf for X is obtained by integrating out y from the joint pdf:

$$\begin{aligned}f_X(x) &= \int_0^\infty \frac{1}{x} e^{-\left(\frac{y}{x}+x\right)}\, \mathrm{d}y = \frac{1}{x} e^{-x} \left(\int_0^\infty e^{-\frac{y}{x}}\, \mathrm{d}y \right) \\ &= \frac{1}{x} e^{-x} \left[-x e^{-\frac{y}{x}} \right]_0^\infty = e^{-x} \left[-e^{-\frac{y}{x}} \right]_0^\infty = e^{-x}\end{aligned}$$

which can be recognized as the density of the exponential distribution with parameter $\beta = 1$. So, marginally we have $X \sim \text{Expon}(1)$.

Conditional distributions for continuous variables

Conditional distribution of Y given $X = x$:

$$f_{Y|X}(y|x) = \frac{f(x,y)}{f_X(x)} \tag{7.12}$$

provided that $f_X(x) > 0$. The conditional distribution of X given $Y = y$ is defined in the same way as

$$f_{X|Y}(x|y) = \frac{f(x,y)}{f_Y(y)} \tag{7.13}$$

provided that $f_Y(y) > 0$.

EXAMPLE: We revisit the joint pdf $f(x,y) = 6x^2y$ for $0 < x < 1, 0 < y < 1$. The marginal pdf for X was earlier found to be $f_X(x) = 3x^2$, for $0 < x < 1$. Hence the conditional density for Y given $X = x$ is given by

$$f_{Y|X}(y|x) = \frac{f(x,y)}{f_X(x)} = \frac{6x^2y}{3x^2} = 2y, \quad 0 < y < 1.$$

Similarly, the marginal pdf for Y was earlier found to be $f_Y(y) = 2y$, for $0 < y < 1$. Hence the conditional density for X given $Y = y$ is given by

$$f_{X|Y}(x|y) = \frac{f(x,y)}{f_Y(y)} = \frac{6x^2y}{2y} = 3x^2, \quad 0 < x < 1.$$

EXAMPLE: Revisit the joint pdf for two continuous random variables X and Y given previously by

$$f(x,y) = \frac{1}{x} e^{-\left(\frac{y}{x} + x\right)}$$

for $0 < x < \infty, 0 < y < \infty$ and $f(x,y) = 0$ otherwise. The marginal pdf for X was found to be $f_X(x) = e^{-x}$. Hence the conditional density for Y given $X = x$ is given by

$$f_{Y|X}(y|x) = \frac{f(x,y)}{f_X(x)} = \frac{\frac{1}{x} e^{-\left(\frac{y}{x} + x\right)}}{e^{-x}} = \frac{1}{x} e^{-\frac{y}{x}}, \quad 0 < y < \infty.$$

Recall that density of the Expon(β) distribution for some variable Y is given by

$$\frac{1}{\beta} e^{-\frac{y}{\beta}}, \quad 0 < y < \infty,$$

where β is the parameter of the distribution. Hence, we can see that $Y|(X = x) \sim \text{Expon}(x)$, i.e. Y given $X = x$ is exponentially distributed with parameter $\beta = x$. This means that the mean of Y given $X = x$ depends on the value obtained for the random variable X.

By reversing (7.12) we see that a joint distribution can be decomposed into a product of a conditional and a marginal distribution:

$$\underbrace{f(x,y)}_{\text{joint}} = \underbrace{f_{Y|X}(y|x)}_{\text{conditional}} \cdot \underbrace{f_X(x)}_{\text{marginal}} \tag{7.14}$$

We will refer to this as the **marginal-conditional decomposition** of a joint distribution. In the previous example we saw that the marginally we have $X \sim \text{Expon}(1)$, and that the conditional distribution for Y given $X = x$ was $Y|X = x \sim \text{Expon}(x)$. This marginal-conditional description of the joint distribution is there more interpretable than the rather cryptic joint distribution

marginal-conditional decomposition

$$f(x,y) = \frac{1}{x} e^{-\left(\frac{y}{x} + x\right)} \qquad \text{for } 0 < x < \infty, 0 < y < \infty.$$

This is how most models are built in practice:

- first specifying a marginal distribution for one variable X
- then specifying a conditional distribution for the other variable Y given $X = x$.

The joint distribution is then automatically obtained from the marginal-conditional decomposition in (7.14). This decomposition is also highly generative: to simulate from the joint distribution $f(x,y)$, we first simulate a realized x from $X \sim \text{Expon}(1)$, and then sample Y from the conditional distribution $Y|(X = x) \sim \text{Expon}(x)$ given that x. Finally, the decomposition makes it also straightforward to change parts of the model. Perhaps a scatter plot of the data suggests that the conditional distribution $Y|(X = x) \sim \text{Expon}(x)$ is not a good fit. We can then easily replace the conditional distribution with the more general Gamma distribution.

7.3 *Independent random variables*

Recall that two events A and B are *independent* if the occurrence of one event does not affect the probability of the other event. This means that a conditional probability is equal to the marginal probability:

$$\Pr(A|B) = \Pr(A) \quad \text{and} \quad \Pr(B|A) = \Pr(B) \tag{7.15}$$

Alternatively, two events A and B are independent if and only if the joint probability of the two events is equal to the product of their

marginal probabilities:

$$\Pr(A \cap B) = \Pr(A) \cdot \Pr(B) \tag{7.16}$$

The same definition applies to random variables:

Definition. *Two discrete random variables X and Y are* independent *if and only if*

$$p_{Y|X}(y|x) = p_Y(y) \tag{7.17}$$

and similarly

$$p_{X|Y}(x|y) = p_X(x) \tag{7.18}$$

Alternatively, X and Y are independent if and only if the joint distribution is equal to the product of the marginal distributions:

$$p(x, y) = p_X(x) \cdot p_Y(y) \tag{7.19}$$

The two variables in the dice rolling experiment, $X =$ number of fives and $Y =$ sum of two dice, are not independent. This can be seen from Figure 7.4, where it is clear that the conditional distribution $p_{X|Y}(x|y)$ is different from the marginal distribution of X; learning about Y tells us something about X. It is quite easy to disprove independence since the property $p(x, y) = p_X(x) \cdot p_Y(y)$ must hold for *all* values of x and y. So we only need to find a single pair of x and y where the property does not hofl in order to show that two variables are not indepedent, that is that they are dependent. For example, in the rolling of the two dice we have we have $p(1, 10) = 0$ while $p_X(1)p_Y(10) = \frac{10}{36} \cdot \frac{3}{36} > 0$. Hence, the two variables X and Y are dependent.

The definition of independence for continuous random variables replaces the joint and marginal probability functions by joint and marginal densities, so that two continuous variables X and Y are independent if and only if

$$f(x, y) = f_X(x) \cdot f_Y(y). \tag{7.20}$$

Here are two examples.

EXAMPLE: Consider the example above with joint density $f(x, y) = 6x^2y$ for $0 < x < 1$ and $0 < y < 1$. The marginal density for X was found to be $f_X(x) = 3x^2$ for $0 < x < 1$ and the marginal density for Y was found to be $f_Y(y) = 2y$ for $0 < y < 1$. The two variables are independent since the joint density is the product of marginal densities:

$$f_X(x)f_Y(y) = 3x^2 \cdot 2y = 6x^2y = f(x, y).$$

Alternatively, we also saw that the conditional distribution for $Y|X$ was $f_{Y|X}(y|x) = 2y$ which was also the marginal distribution for Y; Hence, X carries no information for Y and the two variables are independent.

EXAMPLE: Consider the joint pdf for two continuous random variables X and Y given previously by $f(x,y) = \frac{1}{x}e^{-\left(\frac{y}{x}+x\right)}$ for $0 < x < \infty, 0 < y < \infty$. The conditional distribution $Y|(X = x) \sim \text{Expon}(x)$ clearly depends on x and can therefore not be same as the marginal $f_Y(y)$. Hence, X and Y are dependent.

In the above examples we had to calculcate the marginal distributions in order to check for independence. That is actually not necessary as the following theorem shows.

Theorem 11. *Two continuous random variables X and Y, with rectangular support $(x,y) \in [a,c] \times [c,d]$ for constants a, b, c and d, are independent if and only if the joint distribution can be factorized into a product of two non-negative functions $g(x)$ and $h(y)$,*

$$f(x,y) = g(x) \cdot h(y) \tag{7.21}$$

Note that the functions $g(x)$ and $h(y)$ in the theorem do not need to be densities; if they happen to be densities, then they correpond to the marginal densities $f_X(x)$ and $f_Y(y)$, respectively.

EXAMPLE: The joint density $f(x,y) = 6x^2y$ for $0 < x < 1$ and $0 < y < 1$ can be factorized as $f(x,y) = g(x)h(y)$ where $g(x) = 6x^2$ and $h(y) = y$. Hence, the two variables are independent. Note that there are several other ways to factorize the joint density into a product of two non-negative functions. For example, we could have factorized using the marginal densities $g(x) = f_X(x) = 3x^2$ and $h(y) = f_Y(y) = 2y$. The point is that we do not *need* to find the marginal densities to show that the two variables are independent; as long as we can find some factorization of the joint density into a product of two non-negative functions, then the two variables are independent.

It is important to note the requirement of a rectangular support for the joint density. If the support is non-rectangular, then the support of X depends on the value of Y or vice versa. Such variable cannot be independent, even if their joint density factorizes. For example, X and Y with joint density $f(x,y) = 10x^2y$ for $0 < x < 1$ and $0 < y < x$ (note that the support of Y depends on x) are dependent even thought we can factorize the joint density, for example as $f(x,y) = g(x)h(y)$ where $g(x) = 10x^2$ and $h(y) = y$.

7.4 Covariance and Correlation

covariance

The **covariance** between two random variables X and Y is a measure of *comovement* or *covariation* between the two variables, i.e. the extent to which the two variables move together. We have the following definition.

Definition. *The **covariance** between two random variables X and Y is defined as*

$$\mathbb{C}(X,Y) = \mathbb{E}\big((X-\mu_X)(Y-\mu_Y)\big),$$

where the expectation is with respect to the joint distribution of X and Y, and $\mu_X = \mathbb{E}(X)$ and $\mu_Y = \mathbb{E}(Y)$ are the respective means.

To explain the particular form of covariance, consider first the case with positive comovement between the two variables: whenever X is larger than its mean μ_X also Y tends to be larger than its mean μ_Y, and whenever X is smaller than its mean also Y tends to be smaller than its mean. In both these case we have that so $(X-\mu_X)(Y-\mu_Y)$ is positive with large probability, since the two negative signs cancel when both variables are lower than their respective means; so the covariance is positive when there is positive comovement. With negative comovement we have that whenever X is larger than its mean, Y tends to be *lower* than its mean, so $(X-\mu_X)(Y-\mu_Y)$ is negative, and whenever X is lower than its mean, Y tends to be higher than its mean, so $(X-\mu_X)(Y-\mu_Y)$ is again negative; hence the covariance is negative. This is illustrated in Figure where the blue areas (quadrants) have positive contributions $(X-\mu_X)(Y-\mu_Y) > 0$ to the covariance, and the yellow/beige areas have negative contributions $(X-\mu_X)(Y-\mu_Y) < 0$.

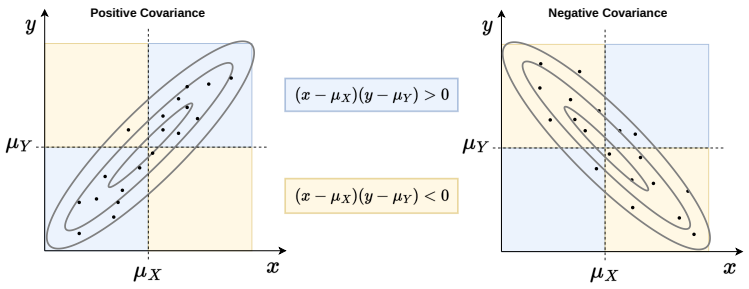

Figure 7.7: Illustration of positive and negative correlation. The blue regions where $(X-\mu_X)(Y-\mu_Y) > 0$ contributes positively to the covariance, while the yellow regions where $(X-\mu_X)(Y-\mu_Y) < 0$ contributes negatively.

The covariance measure in Figure 7.4 depends on the scales of the variables X and Y and may therefore be hard to interpret. For example, changing the scale of measurement from meters to centimeters would lead to a 100 times increase in the covariance. A scale-free,

normalized, version of the covariance is the **correlation coefficient** ρ_{XY} which always lies in the interval $[-1, 1]$. Here is the definition:

correlation coefficient

Definition. *The **correlation** between two random variables X and Y is defined as*

$$\rho_{XY} = \frac{\mathbb{C}(X, Y)}{\sigma_X \cdot \sigma_Y}$$

where σ_X and σ_Y are the standard deviations of X and Y, respectively.

Example: Consider the joint distribution of X and Y given in Table 7.1. The covariance between X and Y is given by

$$\mathbb{C}(X, Y) = \mathbb{E}\big((X - \mu_X)(Y - \mu_Y)\big) = \sum_{x=0}^{2} \sum_{y=2}^{12} (x - \mu_X)(y - \mu_Y) p(x, y)$$

where the mean of X is

$$\mu_X = \sum_{x=0}^{2} x \cdot p_X(x) = 0 \cdot \frac{25}{36} + 1 \cdot \frac{10}{36} + 2 \cdot \frac{1}{36} = \frac{12}{36} = \frac{1}{3}$$

and the mean of Y is

$$\mu_Y = \sum_{y=2}^{12} y \cdot p_Y(y) = 2 \cdot \frac{1}{36} + 3 \cdot \frac{2}{36} + 4 \cdot \frac{3}{36} + \ldots + 11 \cdot \frac{2}{36} + 12 \cdot \frac{1}{36} = 7.$$

The covariance is

$$\begin{aligned}
\mathbb{C}(X, Y) &= \sum_{x=0}^{2} \sum_{y=2}^{12} (x - \mu_X)(y - \mu_Y) p(x, y) \\
&= \sum_{x=0}^{2} \sum_{y=2}^{12} (x - \frac{1}{3})(y - 7) p(x, y) \\
&= \left(0 - \frac{1}{3}\right)(2 - 7)\,\frac{1}{36} + \left(0 - \frac{1}{3}\right)(3 - 7)\,\frac{2}{36} + \ldots \\
&\quad + \left(2 - \frac{1}{3}\right)(12 - 7)\,\frac{0}{36} = 0.5
\end{aligned}$$

The variance of X is given by

$$\mathbb{V}(X) = \sum_{x=0}^{2} (x - \mu_X)^2 \cdot p_X(x) = \frac{25}{36}\left(0 - \frac{1}{3}\right)^2 + \frac{10}{36}\left(1 - \frac{1}{3}\right)^2 + \frac{1}{36}\left(2 - \frac{1}{3}\right)^2 \approx \frac{10}{36}$$

and the variance of Y is given by

$$\mathbb{V}(Y) = \sum_{y=2}^{12} (y - \mu_Y)^2 \cdot p_Y(y) = \frac{1}{36}(2 - 7)^2 + \ldots + \frac{1}{36}(12 - 7)^2 \approx \frac{210}{36}$$

The correlation between X and Y is therefore

$$\rho_{XY} = \frac{\mathbb{C}(X,Y)}{\sigma_X \sigma_Y} = \frac{0.5}{\sqrt{\frac{10}{36}} \cdot \sqrt{\frac{210}{36}}} \approx 0.393.$$

The correlation between these two variables is positive, but only moderately strong.

EXAMPLE: Consider the joint distribution of X and Y given by $f(x,y) = 6x^2y$ for $0 \leq x \leq 1$ and $0 \leq y \leq 1$ with marginal distributions $f_X(x) = 3x^2$ and $f_Y(y) = 2y$. The mean of X is

$$\mu_X = \int_0^1 x \cdot f_X(x)\,\mathrm{d}x = \int_0^1 x \cdot 3x^2\,\mathrm{d}x = 3\left[\frac{x^4}{4}\right]_0^1 = \frac{3}{4}$$

and the mean of Y is

$$\mu_Y = \int_0^1 y \cdot f_Y(y)\,\mathrm{d}y = \int_0^1 y \cdot 2y\,\mathrm{d}y = 2\left[\frac{y^3}{3}\right]_0^1 = \frac{2}{3}.$$

The covariance is then given by

$$\begin{aligned}
\mathbb{C}(X,Y) &= \int_0^1 \int_0^1 (x-\mu_X)(y-\mu_Y) f(x,y)\,\mathrm{d}y\,\mathrm{d}x \\
&= \int_0^1 \int_0^1 (x-\tfrac{3}{4})(y-\tfrac{2}{3}) 6x^2 y\,\mathrm{d}y\,\mathrm{d}x \\
&= 6\int_0^1 (x-\tfrac{3}{4})x^2 \left(\int_0^1 (y-\tfrac{2}{3}) y\,\mathrm{d}y\right)\mathrm{d}x \\
&= 6\int_0^1 (x-\tfrac{3}{4})x^2 \left[\frac{y^3}{3} - \frac{2}{3}\cdot\frac{y^2}{2}\right]_0^1 \mathrm{d}x \\
&= 6\int_0^1 (x-\tfrac{3}{4})x^2 \left(\frac{1}{3} - \frac{1}{3}\right)\mathrm{d}x = 0.
\end{aligned}$$

This example illustrates a general result: **If X and Y are independent, then $\rho_{XY} = 0$.** This is easily verified by using the definition of covariance:

$$\begin{aligned}
\mathbb{C}(X,Y) &= \mathbb{E}\big((X-\mu_X)(Y-\mu_Y)\big) \\
&= \iint (x-\mu_X)(y-\mu_Y) p(x,y)\,\mathrm{d}y\,\mathrm{d}x \\
&= \iint (x-\mu_X)(y-\mu_Y) p_X(x) p_Y(y)\,\mathrm{d}y\,\mathrm{d}x \\
&= \left(\int (x-\mu_X) p_X(x)\,\mathrm{d}x\right)\left(\int (y-\mu_Y) p_Y(y)\,\mathrm{d}y\right) \\
&= \mathbb{E}(X-\mu_X)\cdot\mathbb{E}(Y-\mu_Y) = 0 \cdot 0 = 0.
\end{aligned}$$

However, the converse is not true: **zero correlation does not imply independence**. Covariance and correlation only captures *linear* dependence between two random variables, and variables may be dependent in a nonlinear way. Here is an example.

EXAMPLE: Let $X \sim N(0,1)$ and $Y|(X = x) \sim N(x^2, 1)$. Note that this is an example of the marginal-conditional construction of a joint distribution for (X, Y) in (7.14). The covariance and therefore also the correlation can be shown to be zero, but the two variables are clearly not independent since the conditional mean of Y depends on the observed x. The joint density, plotted in Figure 7.8, is somewhat banana shaped.

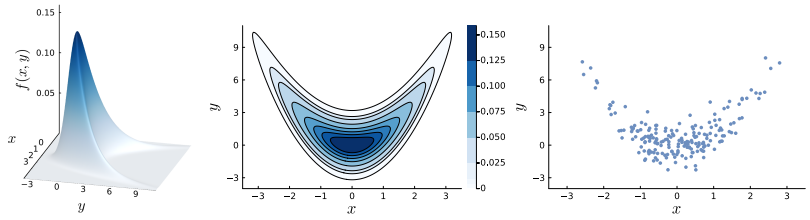

Figure 7.8: The joint density from the model $X \sim N(0,1)$ and $Y|(X = x) \sim N(x^2, 1)$. The left graph plots the joint pdf as a surface while the middle graph plots level contours of the joint pdf, where all (x, y) points on a given contour has the same joint density. The right graph shows a scatter plot of $n = 200$ observations from the joint distribution.

7.5 *Mean, variance and covariance of linear combinations of random variables*

The covariance between random variables is crucial for the variance of a linear combination of dependent random variables, as shown in the following theorem.

Theorem 12. ***Linear combination of two variables***
Let X and Y be two random variables. We then have

$$\mathbb{E}(aX + bY) = a\mathbb{E}(X) + b\mathbb{E}(Y)$$

and

$$\mathbb{V}(aX + bY) = a^2\mathbb{V}(X) + b^2\mathbb{V}(Y) + 2ab\mathbb{C}(X, Y),$$

where a and b are constants and $\mathbb{C}(X, Y)$ is the covariance between X and Y.

When the random variables are independent, the covariance term vanishes and we have the following result

$$\mathbb{V}(aX + bY) = a^2\mathbb{V}(X) + b^2\mathbb{V}(Y).$$

and in the special case with $a = b = 1$ we obtain the variance of the sum of two independent variables which we obtained already in Chapter X

$$\mathbb{V}(X + Y) = \mathbb{V}(X) + \mathbb{V}(Y).$$

When variables are positively correlated, the variance of the sum is larger than the sum of the variances. When two variables tend to co-move together the variance of the sum is naturally larger; a good example is a stock portfolio with two stocks in the same industry. When the price of one stock goes up, the price of the other stock tends to go up as well, and the variance of the portfolio (the sum) is larger than the sum of the stocks' variances. Conversely, when two variables are negatively correlated, the variance of the sum is smaller than the sum of the variances; when one stock goes up, the other stock tends to go down and the variance of the portfolio is smaller than the sum of the variances.

The result in Theorem X can be generalized to a linear combination of more than two random variables.

$$a_1X_1 + a_2X_2, \ldots, a_nX_n = \sum_{i=1}^{n} a_iX_i,$$

where $a_1, a_2, \ldots, a_n$ are constants.

Theorem 13. ***Linear combination of*** n ***variables***
Let $X_1, X_2, \ldots, X_n$ *be* n *random variables. Then*

$$\mathbb{E}\Big(\sum_{i=1}^{n} a_iX_i\Big) = \sum_{i=1}^{n} a_i\mathbb{E}(X_i)$$

and

$$\mathbb{V}\Big(\sum_{i=1}^{n} a_iX_i\Big) = \sum_{i=1}^{n} a_i^2\mathbb{V}(X_i) + 2\sum_{i=1}^{n}\sum_{j=1}^{n} a_ia_j\mathbb{C}(X_i, X_j),$$

where $a_1, a_2, \ldots, a_n$ *are constants.*

Note how all pairwise covariances enter the variance of a linear combination.

7.6 *Iteration laws for conditional expectations and variances*

The **conditional mean** of Y given $X = x$ is defined as conditional mean

$$\mathbb{E}(Y|X = x) = \begin{cases} \sum_y x \cdot p(y|x) & \text{if } x \text{ and } y \text{ discrete} \\ \int y \cdot f(y|x)\mathrm{d}y & \text{if } x \text{ and } y \text{ continuous} \end{cases}$$

It is often the case in many models that calculating the expectation $\mathbb{E}(Y)$ directly is hard, while the conditional expectation $\mathbb{E}(Y|X = x)$ is a much simpler calculation. The following result, the **law of iterated expectation** is useful in this case. To make the notation absolutely clear, we will use the notation $\mathbb{E}_X$ to denote the expectation law of iterated expectation

with respect to the marginal distribution of X, and $\mathbb{E}_{Y|X}$ to denote the expectation with respect to the conditional distribution of Y given $X = x$. The law of iterated expectation states that

Theorem 14. *Law of iterated expectation*

$$\mathbb{E}_Y(Y) = \mathbb{E}_X\big(\mathbb{E}_{Y|X}(Y)\big)$$

The law of iterated expectation therefore corresponds to the following two-step approach:

1. compute the conditional expectation $\mathbb{E}(Y|X)$
2. undo the conditioning on X by taking the expectation $\mathbb{E}_X$.

EXAMPLE: Consider the joint density $f(x, y) = \frac{1}{x} e^{-\left(\frac{y}{x} + x\right)}$ for $x \in (0, \infty)$ and $y \in (0, \infty)$ from a previous example. As we have shown earlier, marginally we have $X \sim \text{Expon}(1)$ and the conditional distribution $Y|(X = x) \sim \text{Expon}(x)$, but the marginal distribution for Y is not so easy to obtain. However, using that the mean in the $\text{Expon}(\beta)$ is β, we known that $\mathbb{E}_{Y|X}(Y) = X$ in the conditional distribution, and $\mathbb{E}_X(X) = 1$; hence, we can use the law of iterated expectation to find the mean of Y:

$$\mathbb{E}(Y) = \mathbb{E}_X\big(\mathbb{E}_{Y|X}(Y)\big) = \mathbb{E}_X(X) = 1.$$

The corresponding result for calculating a marginal variance $\mathbb{V}_Y(Y)$ from a conditional variance $\mathbb{V}_{Y|X}(Y)$ is called the **law of total variance**.

law of total variance

Theorem 15. *Law of total variance*

$$\mathbb{V}_Y(Y) = \mathbb{E}_X\big(\mathbb{V}_{Y|X}(Y)\big) + \mathbb{V}_X\big(\mathbb{E}_{Y|X}(Y)\big)$$

Note the second term, which is easy to forget.

EXAMPLE: Continuing on the previous example, we have $\mathbb{V}_{Y|X}(Y|X) = X^2$ and $\mathbb{E}_{Y|X}(Y) = X$ from properties of the exponential distribution. Hence,

$$\begin{aligned}
\mathbb{V}_Y(Y) &= \mathbb{E}_X\big(\mathbb{V}_{Y|X}(Y)\big) + \mathbb{V}_X\big(\mathbb{E}_{Y|X}(Y)\big) \\
&= \mathbb{E}_X(X^2) + \mathbb{V}_X(X) \\
&= \big(\mathbb{V}_X(X) + (\mathbb{E}_X(X))^2\big) + 1^2 \\
&= \big(1^2 + 1^2\big) + 1^2 = 3
\end{aligned}$$

where we have used that $\mathbb{E}_X(X^2) = \mathbb{V}_X(X) + (\mathbb{E}_X(X))^2$ for any random variable X with mean $\mathbb{E}_X(X)$ and variance $\mathbb{V}_X(X)$.

7.7 *Multivariate random variables**

All of the above concepts with joint, marginal and conditional distributions can be genererlized to more than two random variables. Let $X_1, X_2, \ldots, X_n$ be n random variables. The joint cumulative distribution function is then

$$F(x_1, x_2, \ldots, x_n) = \Pr(X_1 \leq x_1, X_2 \leq x_2, \ldots, X_n \leq x_n)$$

The joint probability density function

$$f(x_1, x_2, \ldots, x_n)$$

is a non-negative function $f(x_1, x_2, \ldots, x_n) \geq 0$ that integrates to one over the support of all n variables

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f(x_1, x_2, \ldots, x_n) \, \mathrm{d}x_1 \, \mathrm{d}x_2 \cdots \mathrm{d}x_n = 1.$$

We can define the *marginal distribution of* X_1, by integrating the joint pdf with respect to all other variables

$$p_{X_1}(x_1) = \underbrace{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty}}_{n-1 \text{ integrals, all except } x_1} f(x_1, x_2, \ldots, x_n) \, \mathrm{d}x_2 \cdots \mathrm{d}x_n$$

We can similarly obtain the marginal distribution for any of the other variables. The marginal distribution of X_2 is obtained by integrating out $X_1, X_3, \ldots, X_n$ and so on. We can even obtain the marginal distribution for any pair of variables, for example the distribution of X_1 and X_2

$$p_{X_1,X_2}(x_1, x_2) = \underbrace{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty}}_{n-2 \text{ integrals, all except } x_1 \text{ and } x_2} f(x_1, x_2, \ldots, x_n) \, \mathrm{d}x_3 \cdots \mathrm{d}x_n$$

The conditional distribution for one variable given all the other variables is called the *full conditional distribution* as is naturally defined as

$$f(x_1 | x_2, \ldots, x_n) = \frac{f(x_1, x_2, \ldots, x_n)}{f(x_2, \ldots, x_n)}$$

where we no longer use subscripts to denote the variables in the distribution, but instead infer those from the rest of the notation, to simplify notation. For example, $f(x_2, \ldots, x_n)$ is the joint distribution for the $n - 1$ variables $X_2, \ldots, X_n$ with X_1 integrated (marginalized) out.

With multiple variables, the notation quickly becomes rather cumbersome. It is convenient to switch to a notation based on vectors; see Section 1.18 for an introduction to vectors and matrices. We use bold

letters to denote vectors, for example $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ is vector containing the n random variables, and $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ is a vector with realized values for those n variables. The joint pdf for all n variables can then be expressed simply as $f(\mathbf{x})$ which means exactly the same things as the more lengthy $f(x_1, x_2, \ldots, x_n)$. Similarly, we can write $F(\mathbf{x})$ for the joint cdf. For example, to be very concrete, with $n = 3$ we can write

$$F(2, 1, 0) = \Pr(X_1 \leq 2, X_2 \leq 1, X_3 \leq 0)$$

simply as $F(\mathbf{x})$ where $\mathbf{x} = (2, 1, 0)^\top$. Note the use of the *transpose* $^\top$, which is not strictly necessary, but makes $\mathbf{x}$ into a *column vector*,

$$\mathbf{x} = (2, 1, 0)^\top = \begin{pmatrix} 2 \\ 1 \\ 0 \end{pmatrix},$$

which is a common convention.

Let us split up the elements of a vector $\mathbf{X} = (X_1, X_2, \ldots, X_n)^\top$ in two shorter vectors

$$\mathbf{X} = \begin{pmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{pmatrix}$$

where $\mathbf{X}_1$ is a vector with the first n_1 elements of $\mathbf{X}$ and $\mathbf{X}_2$ is vector with the last $n_2 = n - n_1$ elements of $\mathbf{x}$. We can then write the marginal distribution of the first n_1 random variables in $\mathbf{X}$ as $f(\mathbf{x}_1)$ and the distribution of the first n_1 variables in $\mathbf{X}_1$ conditional on the remaining n_2 variables in $\mathbf{X}_2$ as

$$f(\mathbf{x}_1|\mathbf{x}_2) = \frac{f(\mathbf{x}_1, \mathbf{x}_2)}{f(\mathbf{x}_2)}.$$

As a concrete example, let $\mathbf{X}$ contain $n = 4$ random variables divided into $n_1 = 2$ variables in $\mathbf{X}_1$ and the remaining $n_2 = 2$ variables in $\mathbf{X}_2$. The density in the point $x_1 = 1, x_2 = 3$ conditional on $x_3 = 5, x_4 = 0$ is then $f(\mathbf{x}_1|\mathbf{x}_2) = f((1, 3)|(5, 0))$.

In an earlier section, we presented formulas for computing the mean and variance of a linear combination of random variables. These formulas can be written much more compactly using vector notation. Let $\mathbf{X} = (X_1, X_2, \ldots, X_n)^\top$ be a column vector containing all n random variables. Similarly, let $\mathbf{a} = (a_1, a_2, \ldots, a_n)^\top$ be a vector with the constants in the linear combination. Note that the linear combination can be written as the vector product

$$\mathbf{a}^\top \mathbf{X} = (a_1, \ldots, a_n) \begin{pmatrix} \mathbf{X}_1 \\ \vdots \\ \mathbf{X}_n \end{pmatrix} = \sum_{i=1}^{n} a_i X_i.$$

Finally, let $\mathbf{\Sigma}$ be the $n \times n$ covariance matrix

$$\mathbf{\Sigma} = \begin{pmatrix} \mathbb{V}(X_1) & \mathbb{C}(X_1, X_2) & \dots & \mathbb{C}(X_1, X_n) \\ \mathbb{C}(X_2, X_1) & \mathbb{V}(X_2) & \dots & \mathbb{C}(X_2, X_n) \\ \vdots & \vdots & \ddots & \vdots \\ \mathbb{C}(X_n, X_1) & \mathbb{C}(X_n, X_2) & \dots & \mathbb{V}(X_n) \end{pmatrix}$$

containing the variances of the variables on the diagonal and pairwise covariances on the off-diagonal positions. We can now express the mean and variance of a linear combination of n random variables compactly as

$$\mathbb{E}(\mathbf{a}^\top \mathbf{X}) = \mathbf{a}^\top \boldsymbol{\mu} \tag{7.22}$$

$$\mathbb{V}(\mathbf{a}^\top \mathbf{X}) = \mathbf{a}^\top \mathbf{\Sigma} \mathbf{a} \tag{7.23}$$

where $\boldsymbol{\mu} = \mathbb{E}(\mathbf{X})$ is the vector with the means of the random variables.

EXERCISES

Joint distributions

1. Let $f(x, y) = cx^2$ be a joint density for X and Y, where c is constant. Determine the constant c.
2. Show that $f(x, y) = 10x^2 y$ for $0 < x < 1$ and $0 < y < x$ and $f(x, y) = 0$ otherwise is a valid joint density function.

8 Likelihood inference

8.1 Probability, Inference, Prediction and Decisions

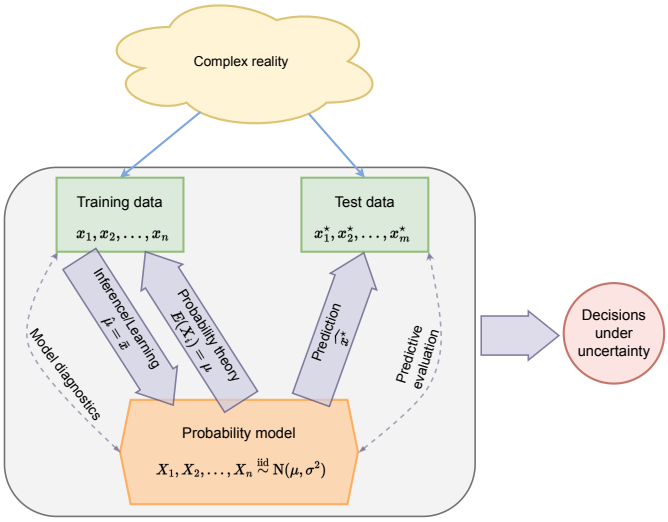

Figure 8.1: The big picture of statistics: probability, inference, prediction and decisions.

8.2 The likelihood function

8.3 Maximum likelihood

$$\hat{\theta} = \arg\max_{\theta \in \Theta} p(y_1, y_2, \ldots, y_n | \theta) \tag{8.1}$$

MLE for Bernoulli data

Consider a sample of n independent and identically distributed (iid) observations from a Bernoulli distribution with parameter θ:

$$X_1, X_2, \ldots, X_n \sim \text{Bern}(\theta) \tag{8.2}$$

$$P(x_1, x_2, \ldots, x_n | \theta) = \prod_{i=1}^{n} P(x_i | \theta) \tag{8.3}$$

$$\ell(\theta) = \log P(x_1, x_2, \ldots, x_n|\theta) = \sum_{i=1}^{n} \log P(x_i|\theta) \tag{8.4}$$

In the case where data comes from a Bernoulli distribution, the probability function for an observation is simply $P(x) = \theta^x(1-\theta)^{1-x}$. Because of independence, the likelihood function is therefore the product

$$P(x_1, x_2, \ldots, x_n|\theta) = \prod_{i=1}^{n} \theta^{x_i}(1-\theta)^{1-x_i} = \theta^s(1-\theta)^{n-s}, \tag{8.5}$$

where $s = \sum_{i=1}^{n} x_i$ is the number of successes in the sample. Hence, the log-likelihood function is

$$\ell(\theta) = s \log \theta + (n-s) \log(1-\theta). \tag{8.6}$$

We know from mathematical analysis that the maximum of a function $f(x)$ is found by setting the first derivative to zero and solving for x. The first derivative of the log-likelihood is

$$\frac{d}{d\theta}\ell(\theta) = \frac{s}{\theta} - \frac{n-s}{1-\theta} \tag{8.7}$$

Setting the first derivative to zero

$$\frac{s}{\theta} - \frac{n-s}{1-\theta} = 0 \tag{8.8}$$

and solving for θ gives the solution $\theta = s/n$, the fraction of successes in the sample. We can verify that this is indeed a maximum by checking whether the second derivative is negative at $\theta = s/n$. The second derivative is

$$\frac{d^2}{d\theta^2}\ell(\theta) = -\frac{s}{\theta^2} - \frac{n-s}{(1-\theta)^2} \tag{8.9}$$

which is negative for all θ.

MLE for Poisson data

$$X_1, X_2, \ldots, X_n|\theta \overset{\text{iid}}{\sim} \text{Pois}(\lambda) \tag{8.10}$$

$$\ell(\lambda) = \log L(\lambda) = \log P(x_1, x_2, \ldots, x_n|\lambda) = \sum_{i=1}^{n} \log P(x_i|\lambda) \tag{8.11}$$

In the case where data comes from a Poisson distribution, the probability function for an observation is

$$P(x) = \frac{e^{-\lambda}\lambda^x}{x!} \tag{8.12}$$

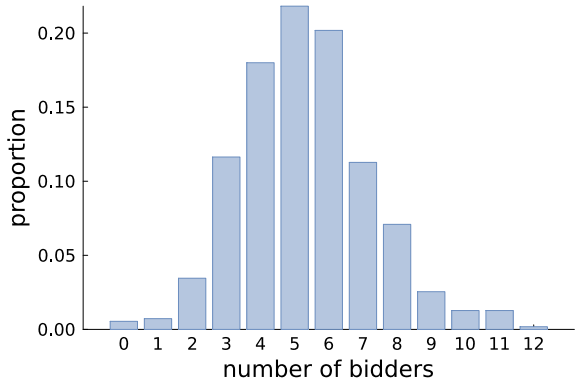

Figure 8.2: The number of bidders in $n = 550$ eBay coin auctions with low reservation price.

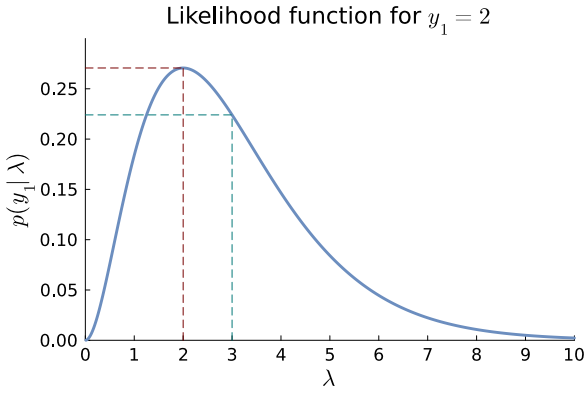

Figure 8.3: Likelihood function $p(y_1|\lambda)$ for the first observation $y_1 = 2$ in the eBay data.

and therefore

$$\log P(x) = -\lambda + x \log \lambda - \log x! \tag{8.13}$$

so the log-likelihood function is

$$\ell(\lambda) = \sum_{i=1}^{n} \Big(-\lambda + x_i \log \lambda - \log(x_i!) \Big) = -n\lambda + \log \lambda \sum_{i=1}^{n} x_i - \sum_{i=1}^{n} \log(x_i!) \tag{8.14}$$

We know from mathematical analysis that the maximum of a function $f(x)$ is found by setting the first derivative to zero and solving for x. The first derivative has a simple form:

$$\frac{d}{d\lambda} \ell(\lambda) = -n + \frac{\sum_{i=1}^{n} x_i}{\lambda} = 0 \tag{8.15}$$

which gives the solution $\lambda = \frac{\sum_{i=1}^{n} x_i}{n} = \bar{x}$. We can verify that this is indeed a maximum by checking whether the second derivative is negative at $\lambda = \bar{x}$. The second derivative is

$$\frac{d^2}{d\lambda^2} \ell(\lambda) = -\frac{\sum_{i=1}^{n} x_i}{\lambda^2}, \tag{8.16}$$

which is negative for all λ since both the data and λ must be positive. The maximum likelihood estimator of the parameter λ in the univariate Poisson model is therefore the sample mean $\hat{\lambda} = \bar{x}$.

MLE for the iid Normal model

Consider the iid Normal model $Y_1, \ldots, Y_n | \boldsymbol{\theta} \overset{\text{iid}}{\sim} N(\mu, \sigma^2)$, where $\boldsymbol{\theta} = (\mu, \sigma^2)^\top$. This model has two parameters, and we will now show that the maximum likelihood estimator can easily be extended to this case. The definition is the same, but the maximization is now over a vector with d parameters, $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_d)^\top$,

$$\hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} p(y_1, y_2, \ldots, y_n | \boldsymbol{\theta}) \tag{8.17}$$

The maximum of this multi-input function is found by setting the first partial derivatives of the log-likelihood $\ell(\theta_1, \ldots, \theta_d)$ to zero and solving the resulting systems of d equations (see Section 1.15):

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\theta_1} \ell(\theta_1, \ldots, \theta_d) &= 0 \\
\frac{\mathrm{d}}{\mathrm{d}\theta_2} \ell(\theta_1, \ldots, \theta_d) &= 0 \\
&\vdots \\
\frac{\mathrm{d}}{\mathrm{d}\theta_d} \ell(\theta_1, \ldots, \theta_d) &= 0
\end{aligned}$$

If we collect the partial derivatives into a vector, we can write the system of equations as

$$\ell'(\boldsymbol{\theta}) = \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}\ell(\boldsymbol{\theta}) = \mathbf{0} \tag{8.18}$$

The d-element vector with partial derivatives is in general called the gradient, and when applied to the log-loglikelihood $\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}\ell(\boldsymbol{\theta})$ is called the **score vector**.

score vector

The log-likelihood function for the iid Normal model is

$$\begin{aligned}\ell(\boldsymbol{\theta}) &= -\frac{n}{2}\log(2\pi) - \frac{n}{2}\log(\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i-\mu)^2 \\ &= -\frac{n}{2}\log(2\pi) - \frac{n}{2}\log(\phi) - \frac{1}{2\phi}\sum_{i=1}^{n}(y_i-\mu)^2,\end{aligned}$$

where we have defined $\phi = \sigma^2$, since it will simplify the notation without having the square to move around when taking derivatives. The partial derivatives of the log-likelihood function are

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\mu}\ell(\boldsymbol{\theta}) &= -\frac{1}{2\phi}2\sum(y_i-\mu)\cdot(-1) = \frac{1}{\phi}n(\bar{y}-\mu) \\ \frac{\mathrm{d}}{\mathrm{d}\phi}\ell(\boldsymbol{\theta}) &= -\frac{n}{2}\frac{1}{\phi} + \frac{1}{2\phi^2}\sum(y_i-\mu)^2.\end{aligned}$$

The equation $\frac{\mathrm{d}}{\mathrm{d}\mu}\ell(\boldsymbol{\theta}) = \frac{1}{\phi}n(\bar{y}-\mu) = 0$ has solution $\hat{\mu} = \bar{y}$. Inserting this maximizer in the second equation gives

$$\frac{\mathrm{d}}{\mathrm{d}\phi}\ell(\boldsymbol{\theta}) = -\frac{n}{2}\frac{1}{\phi} + \frac{1}{2\phi^2}\sum(y_i-\bar{y})^2 = 0$$

which has solution $\hat{\phi} = \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i-\bar{y})^2$. We return to this example in Section 8.4 where it is shown that this indeed a maximum by the second derivative test.

Note that the MLE for σ^2 is not the usual unbiased estimator of the variance $s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(y_i-\bar{y})^2$, and the MLE for σ^2 is biased. The bias vanishes however when $n \to \infty$ and we will later see that this *asympotically unbiased* property of the MLE is true for essentially any model.

EXERCISES

Maximum likelihood

1. Let $X_1, \ldots, X_n|\theta \overset{\text{iid}}{\sim} \text{Expon}(\theta)$ be iid exponentially distributed survival times of patients after a cancer treatment. Derive the maximum likelihood estimator for θ.

2. Luckily, some patients were still alive at the end of the study. This means that the exact life times for surviving patients is unknown, but we do know that they lived *at least* the time recorded at the end of the study. We say that their data are *censored*. Derive the maximum likelihood estimator for θ when n_c of the n observations are censored.

8.4 Observed and Expected information

It is often of interest to know how much information the data provides about the parameter θ, i.e. how much we have learned about the unknown parameter from observing a dataset. The following definition, based on the second derivative of the log-likelihood function, may seem a bit strange at first, but it is actually quite intuitive. Here is the definition of the **observed information**:

observed information

Definition. *The **observed information** about a model parameter θ from a sample of size n is defined as*

$$\mathcal{J}_n(\hat{\theta}) = -\ell''(\hat{\theta}) = -\frac{\mathrm{d}^2}{\mathrm{d}\theta^2}\ell(\theta) \mid_{\theta=\hat{\theta}} \tag{8.24}$$

So, why is the second derivative of the log-likelihood function a measure of information? Recall from Section 1.14 that the first derivative measures the local slope of the function at some point. The second derivative measures the change in the first derivative, i.e. how quickly the slope is changing. If the slope is changing quickly, then the function is curving sharply, and we can be more certain about the value of the parameter θ. In other words, if the second derivative, and therefore the observation information, is large, then we have a lot of information about θ. Conversely, if the second derivative is small, then we have little information about θ. The reason for the negative sign is that the second derivative is negative at the maximum likelihood estimate $\hat{\theta}$, so by multiplying by -1 we ensure that the observed information is positive.

EXAMPLE: IID POISSON. Let $Y_1, \ldots, Y_n|\theta$ be a sample from a Poisson distribution with parameter λ. As shown in Section 8.3, the log-likelihood function is

$$\ell(\lambda) = -n\lambda + \log\lambda \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} \log(y_i!)$$

with MLE $\theta = \bar{y}$ and second derivative

$$\ell''(\lambda) = -\frac{\sum_{i=1}^{n} y_i}{\lambda^2} = -\frac{n\bar{y}}{\lambda^2}$$

so the observed information is

$$\mathcal{J}_n(\bar{y}) = -\ell''(\bar{y}) = \frac{n\bar{y}}{\bar{y}^2} = \frac{n}{\bar{y}},$$

which increases linearly with the sample size n.

The observed information varies from sample to sample. The **expected information**, also called the **Fisher information**, is defined average information over all possible datasets of size n:

expected information

Fisher information

Definition. *The Fisher information is the expected value of the observed information at the parameter value θ, i.e.*

$$\mathcal{I}_n(\theta) = \mathbb{E}\left(\mathcal{J}_n(\theta)\right). \tag{8.25}$$

where the expectation is taken with respect to the sampling distribution of the data $Y_1, \ldots, Y_n|\theta$.

The Fisher information has at least five important uses:

- First, before the data is collected, it measures how much information the data is *expected* to provide about the parameter θ; this makes the Fisher information useful when **designing experiments**.

designing experiments

- Second, the Fisher information can be used to measure the repeated sampling variability of the maximum likelihood estimator $\hat{\theta}$, as we will show in the next section.
- Third, the famous **Cramér–Rao bound** says that inverse Fisher information is the smallest possible sampling variance of *any* unbiased estimator.

Cramér–Rao bound

- Fourth, the Fisher information appears in Jeffreys' prior, a particular type of invariant prior using in Bayesian learning; see (Villani, 2025) for more details.
- Finally, and most important for Bayesian theory, is that the posterior distribution in large samples involves the Fisher information (Villani, 2025).

Example: iid Poisson. The Fisher information is here given by

$$\mathcal{I}_n(\lambda) = -\mathbb{E}\left(\ell''(\lambda)\right) = \mathbb{E}\left(\frac{\sum_{i=1}^n Y_i}{\lambda^2}\right) = \left(\frac{\sum_{i=1}^n \mathbb{E}(Y_i)}{\lambda^2}\right) = \frac{n\lambda}{\lambda^2} = \frac{n}{\lambda},$$

since $\mathbb{E}(Y_i) = \lambda$ for a Poisson random variable.

EXERCISES

Observed and Fisher information

1. Let $Y_1, \ldots, Y_n|\theta$ be a sample from an Bernoulli distribution with parameter p. Compute the observed information $\mathcal{J}_n(\hat{p})$ and the Fisher information $\mathcal{I}_n(p)$.
2. Compute the observed information $\mathcal{J}_n(\hat{\theta})$ and the Fisher information $\mathcal{I}_n(\theta)$ for the exponential model.

8.5 Sampling distribution of the MLE

The role of the Fisher information $\mathcal{I}_n(\theta)$ in measuring uncertainty in the MLE is clearly spelled out in the following theorem, which states that the sampling distribution of the MLE is approximately normal with mean θ and variance $1/\mathcal{I}_n(\theta)$ in large samples.

Theorem 16. *(Asymptotic normality of the MLE - informal)*

$$\hat{\theta}_n(Y_1, \ldots, Y_n) \overset{\text{approx}}{\sim} N\left(\theta, \frac{1}{\mathcal{I}_n(\theta)}\right) \quad \text{as } n \to \infty$$

where it is explicit that the MLE is a function of the data $Y_1, \ldots, Y_n$.

The formal version of this results says that

$$\frac{\hat{\theta}_n - \theta}{\sqrt{\mathcal{I}_n^{-1}(\theta)}} \xrightarrow{d} N(0,1) \quad \text{as } n \to \infty$$

Hence, the standardized MLE *converges in distribution* to a standard normal distribution. A side-effect of the result in Theorem 16 is that the MLE is **asymptotically unbiased**, meaning that $\mathbb{E}(\hat{\theta}_n) = \theta$ as $n \to \infty$.

asymptotically unbiased

The above result for the large sample approximation is not practical since it depends on the unknown parameter value θ. We can replace θ by its MLE, but calculating the expected value in the Fisher information is not always easy, particularly in more complex models. However, in large samples we have $\mathcal{I}_n(\hat{\theta}) \approx \mathcal{J}_n(\hat{\theta})$, and we can use the approximation:

Theorem 17. *(practical approximate sampling distribution for the MLE in large samples)*

$$\hat{\theta}_n(Y_1, \ldots, Y_n) \overset{\text{approx}}{\sim} N\left(\theta, \frac{1}{\mathcal{J}_n(\hat{\theta})}\right) \quad \text{as } n \to \infty$$

This approximation is practically very useful, since even in complex models we can use numerical maximization to find $\hat{\theta}$ and then

compute the second derivative at the MLE using automatic differentiation, or build up an estimate of it as part of the optimization algorithm (e.g. using the so called BFGS algorithm for optimization). All of this can also be extended to the case with more than one parameter, see Section 8.6, where it becomes truly indispensable. The large sample approximation in Theorem 17 is often surprisingly accurate also in quite moderately sized datasets. Finally, the approximation can be used to construct an approximate 95% confidence interval by

$$\hat{\theta} \pm 1.96\sqrt{\mathcal{J}_n^{-1}(\hat{\theta})}$$

or any other confidence level by replacing 1.96 with the appropriate quantile from the standard normal distribution.

It is common to want the maximum likelihood estimate of a *function* $g(\theta)$ of the parameter θ. A very nice property of the maximum likelihood estimator is that it is **equivariant**, meaning that if $\hat{\theta}$ is the MLE for θ, then $g(\hat{\theta})$ is the MLE for $g(\theta)$; that is, we can just plug in the MLE in the function $g(\cdot)$ to get the MLE for the function. We state this important property as a theorem.

equivariant

Theorem 18. *The maximum likelihood estimator (MLE) $\hat{\theta}$ is **equivariant**, i.e. the MLE for any function $g(\theta)$ of the parameter is*

$$\widehat{g(\theta)} = g(\hat{\theta}).$$

Example: iid Bernoulli. Consider the Bernoulli model with probability θ as the parameter. It is quite common to report an estimate of the so called *log-odds*

$$\log\left(\frac{\theta}{1-\theta}\right),$$

which in some applications is easier to interpret; this is particularly true when the Bernoulli model is extended to a regression model in Chapter 9. Since the MLE of θ is $\hat{\theta} = s/n$, the equivariance property of the MLE immediately gives that the MLE for the log-odds is $\log\left(\frac{\hat{\theta}}{1-\hat{\theta}}\right) = \log\left(\frac{s/n}{f/n}\right) = \log(s/f)$.

Theorem 20 says that the sampling distribution of the MLE $\hat{\theta}$ is approximately normal in large samples. An interesting question is then how this sampling distribution carries over to a function $g(\theta)$ of the parameter. Assume first that $g(\theta) = a + b\theta$ is a linear function for constant a and b. By the equivariance of the MLE, the MLE for $g(\theta)$ is $a + b\hat{\theta}$. The mean of the MLE for $g(\theta)$ is then

$$\mathbb{E}(g(\hat{\theta})) = a + b\mathbb{E}(\hat{\theta}).$$

The variance of the MLE for $g(\theta)$ is

$$\mathbb{V}(g(\hat{\theta})) = \mathbb{V}(a + b\hat{\theta}) = b^2\mathbb{V}(\hat{\theta}).$$

Since the MLE is asymptotically unbiased, we have $\mathbb{E}(\hat{\theta}) = \theta$ in large samples. Moreover, we have $\mathbb{V}(\hat{\theta}) \approx \mathcal{J}_n^{-1}(\hat{\theta})$ for large n, and we therefore have the following large sample approximation of the sampling distribution

$$\widehat{g(\theta)}_n(Y_1, \ldots, Y_n) \overset{\text{approx}}{\sim} N\left(a + b\theta,\, b^2\mathcal{J}_n^{-1}(\hat{\theta})\right) \quad \text{as } n \to \infty$$

What about the general case with a potentially non-linear function $g(\theta)$? A heuristic derivation of a large sample approximation of the sampling distribution of $\widehat{g(\theta)}$ uses a first order Taylor approximation (see Section 1.17) of the function around $\hat{\theta}$

$$g(\theta) \approx g(\hat{\theta}) + g'(\hat{\theta})(\theta - \hat{\theta}),$$

where $g'(\hat{\theta})$ is the derivative of $g(\theta)$ evaluated at the MLE $\hat{\theta}$. Since the likelihood becomes more and more concentrated around $\hat{\theta}$ as $n \to \infty$, the Taylor approximation will be accurate for all θ with non-negligible likelihood values. This is the heuristic explaination of the following result.

Theorem 19. *The approximate sampling distribution for the MLE of a function $g(\theta)$ in large samples is*

$$\widehat{g(\theta)}(Y_1, \ldots, Y_n) \overset{\text{approx}}{\sim} N\left(g(\theta),\, g'(\hat{\theta})^2\mathcal{J}_n^{-1}(\hat{\theta})\right) \quad \text{as } n \to \infty$$

8.6 Information and sampling distribution of the MLE - multi-parameter case*

In models with more than one parameter, the observed information becomes an **observed information matrix**. In the case with two parameters $\boldsymbol{\theta} = (\theta_1, \theta_2)^\top$, the observed information matrix is

observed information matrix

$$\mathcal{J}_n(\hat{\boldsymbol{\theta}}) = -\begin{pmatrix} \frac{\mathrm{d}^2}{\mathrm{d}\theta_1^2}\ell(\boldsymbol{\theta}) & \frac{\mathrm{d}^2}{\mathrm{d}\theta_1\,\mathrm{d}\theta_2}\ell(\boldsymbol{\theta}) \\ \frac{\mathrm{d}^2}{\mathrm{d}\theta_2\,\mathrm{d}\theta_1}\ell(\boldsymbol{\theta}) & \frac{\mathrm{d}^2}{\mathrm{d}\theta_2^2}\ell(\boldsymbol{\theta}) \end{pmatrix}\Bigg|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}}$$

i.e. a 2×2 matrix with the second derivatives of the log-likelihood function with respect to the two parameters θ_1 and θ_2 on the diagonal and the partial cross-derivatives $\frac{\mathrm{d}^2}{\mathrm{d}\theta_2\,\mathrm{d}\theta_1}\ell(\boldsymbol{\theta})$ at the off-diagonal elements. All derivatives are evaluated at the maximum likelihood estimate $\hat{\boldsymbol{\theta}} = (\hat{\theta}_1, \hat{\theta}_2)^\top$.

EXAMPLE: IID NORMAL. Consider again the iid Normal model $Y_1, \ldots, Y_n | \boldsymbol{\theta} \overset{\text{iid}}{\sim} N(\mu, \sigma^2)$, where $\boldsymbol{\theta} = (\mu, \sigma^2)^\top$; we will again define $\phi = \sigma^2$ to simplify notation. The partial derivatives of the log-likelihood function were in Section 8.3 shown to be

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\mu}\ell(\boldsymbol{\theta}) &= \frac{1}{\phi} n(\bar{y} - \mu) \\
\frac{\mathrm{d}}{\mathrm{d}\phi}\ell(\boldsymbol{\theta}) &= -\frac{n}{2}\frac{1}{\phi} + \frac{1}{2\phi^2}\sum (y_i - \mu)^2.
\end{aligned}$$

The second partial derivatives and cross-partial derivative of the log-likelihood function are

$$\begin{aligned}
\frac{\mathrm{d}^2}{\mathrm{d}\mu^2}\ell(\boldsymbol{\theta}) &= -\frac{n}{\phi} = -\frac{n}{\sigma^2} \\
\frac{\mathrm{d}^2}{\mathrm{d}\phi^2}\ell(\boldsymbol{\theta}) &= \frac{n}{2\phi^2} - \frac{1}{\phi^3}\sum (y_i - \mu)^2 \\
\frac{\mathrm{d}^2}{\mathrm{d}\mu\,\mathrm{d}\phi}\ell(\boldsymbol{\theta}) &= -\frac{1}{\phi^2} n(\bar{y} - \mu)
\end{aligned}$$

Evaluating these second derivatives at the MLE $\hat{\mu} = \bar{y}$ and $\hat{\phi} = \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^n (y_i - \bar{y})^2$ gives

$$\begin{aligned}
\frac{\mathrm{d}^2}{\mathrm{d}\mu^2}\ell(\boldsymbol{\theta})|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} &= -\frac{n}{\hat{\sigma}^2} \\
\frac{\mathrm{d}^2}{\mathrm{d}\phi^2}\ell(\boldsymbol{\theta})|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} &= \frac{n}{2\hat{\phi}^2} - \frac{1}{\hat{\phi}^3}\sum (y_i - \bar{y})^2 = \frac{n}{2\hat{\phi}^2} - \frac{1}{\hat{\phi}^3} n\hat{\phi} = -\frac{n}{2\hat{\phi}^2} = -\frac{n}{2\hat{\sigma}^4} \\
\frac{\mathrm{d}^2}{\mathrm{d}\mu\,\mathrm{d}\phi}\ell(\boldsymbol{\theta})|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} &= 0
\end{aligned}$$

The observed information matrix is therefore

$$\mathcal{J}_n(\hat{\boldsymbol{\theta}}) = -\begin{pmatrix} -\frac{n}{\hat{\sigma}^2} & 0 \\ 0 & -\frac{n}{2\hat{\sigma}^4} \end{pmatrix} = \begin{pmatrix} \frac{n}{\hat{\sigma}^2} & 0 \\ 0 & \frac{n}{2\hat{\sigma}^4} \end{pmatrix}$$

To calculate the Fisher information matrix, we need the expected value of the second derivatives

$$\begin{aligned}
\mathbb{E}\left(\frac{\mathrm{d}^2}{\mathrm{d}\mu^2}\ell(\boldsymbol{\theta})\right) &= -\frac{n}{\sigma^2} \\
\mathbb{E}\left(\frac{\mathrm{d}^2}{\mathrm{d}\phi^2}\ell(\boldsymbol{\theta})\right) &= \frac{n}{2\phi^2} - \frac{1}{\phi^3}\sum \mathbb{E}(Y_i - \mu)^2 = \frac{n}{2\phi^2} - \frac{1}{\phi^3} n\phi = -\frac{n}{2\phi^2},
\end{aligned}$$

since $\mathbb{E}(Y_i - \mu)^2 = \sigma^2 = \phi$, by the definition of the variance. The Fisher information matrix is therefore

$$\mathcal{I}_n(\boldsymbol{\theta}) = \begin{pmatrix} \frac{n}{\sigma^2} & 0 \\ 0 & \frac{n}{2\phi^2} \end{pmatrix} = \begin{pmatrix} \frac{n}{\sigma^2} & 0 \\ 0 & \frac{n}{2\sigma^4} \end{pmatrix}$$

Now that we have made the effort to compute the matrix of second partial derivatives, the so called *Hessian matrix*

$$\frac{\mathrm{d}^2}{\mathrm{d}\boldsymbol{\theta}\,\mathrm{d}\boldsymbol{\theta}^\top}\ell(\boldsymbol{\theta}) = \begin{pmatrix} -\frac{n}{\sigma^2} & 0 \\ 0 & -\frac{n}{2\sigma^4} \end{pmatrix},$$

we can verify that the solution $\hat{\mu} = \bar{y}$ and $\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^n (y_i - \bar{y})^2$ is indeed a maximum of the likelihood function. From the second partial derivative test in Section 1.15 we need to check that the determinant of the Hessian is positive at the MLE $\hat{\boldsymbol{\theta}}$, i.e.

$$\left|\frac{\mathrm{d}^2}{\mathrm{d}\boldsymbol{\theta}\,\mathrm{d}\boldsymbol{\theta}^\top}\ell(\boldsymbol{\theta})\right| = \Big(-\frac{n}{\sigma^2}\Big)\Big(-\frac{n}{2\sigma^4}\Big) = \frac{n^2}{2\sigma^6} > 0,$$

for all $\sigma^2 > 0$, and therefore also for $\hat{\sigma}^2$; note that we have used that the determinant of a diagonal matrix is the product of the diagonal elements (see Section 1.18). We also need to check that the second derivative with respect to μ is negative at the maximum likelihood estimate $\hat{\boldsymbol{\theta}}$. Since $\frac{\mathrm{d}^2}{\mathrm{d}\mu^2}\ell(\boldsymbol{\theta}) = -\frac{n}{\sigma^2} < 0$ for all $\sigma^2 > 0$, this is indeed a maximum of the likelihood function.

The **observed information matrix** in the general case with d parameters $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_d)^\top$ follows the same pattern as in the case with two parameter, and is given in the next definition.

observed information matrix

Definition. *The **observed information matrix** is the matrix of second derivatives of the log-likelihood evaluated at the MLE $\hat{\boldsymbol{\theta}}$:*

$$\mathcal{J}_n(\hat{\boldsymbol{\theta}}) = -\begin{pmatrix} \frac{\mathrm{d}^2}{\mathrm{d}\theta_1^2}\ell(\boldsymbol{\theta}) & \frac{\mathrm{d}^2}{\mathrm{d}\theta_1\,\mathrm{d}\theta_2}\ell(\boldsymbol{\theta}) & \cdots & \frac{\mathrm{d}^2}{\mathrm{d}\theta_1\,\mathrm{d}\theta_d}\ell(\boldsymbol{\theta}) \\ \frac{\mathrm{d}^2}{\mathrm{d}\theta_2\,\mathrm{d}\theta_1}\ell(\boldsymbol{\theta}) & \frac{\mathrm{d}^2}{\mathrm{d}\theta_2^2}\ell(\boldsymbol{\theta}) & \cdots & \frac{\mathrm{d}^2}{\mathrm{d}\theta_2\,\mathrm{d}\theta_d}\ell(\boldsymbol{\theta}) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\mathrm{d}^2}{\mathrm{d}\theta_d\,\mathrm{d}\theta_1}\ell(\boldsymbol{\theta}) & \frac{\mathrm{d}^2}{\mathrm{d}\theta_d\,\mathrm{d}\theta_2}\ell(\boldsymbol{\theta}) & \cdots & \frac{\mathrm{d}^2}{\mathrm{d}\theta_d^2}\ell(\boldsymbol{\theta}) \end{pmatrix}\Bigg|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}}$$

The **expected information matrix**, or **Fisher information matrix**, is again the expectation of the observed information matrix with respect to the sampling distribution.

expected information matrix

Fisher information matrix

Definition. *The **Fisher information matrix** is the expected value of the observed information at the parameter value $\boldsymbol{\theta}$, i.e.*

$$\mathcal{I}_n(\boldsymbol{\theta}) = \mathbb{E}\left(\mathcal{J}_n(\boldsymbol{\theta})\right). \tag{8.26}$$

where the expectation is taken with respect to the sampling distribution of the data $Y_1, \ldots, Y_n|\boldsymbol{\theta}$.

Similar to the one-parameter case, we have the following highly practical large sample approximation to the sampling distribution of the maximum likelihood estimator.

Theorem 20. *The approximate sampling distribution for the MLE for a parameter vector $\boldsymbol{\theta}$ in large samples is multivariate normal*

$$\hat{\boldsymbol{\theta}}_n(Y_1, \ldots, Y_n) \overset{\text{approx}}{\sim} N\left(\boldsymbol{\theta}, \mathcal{J}_n^{-1}(\hat{\boldsymbol{\theta}})\right) \quad \text{as } n \to \infty,$$

where $\mathcal{J}_n^{-1}(\hat{\boldsymbol{\theta}})$ is the $d \times d$ matrix inverse of the observed information matrix.

The equivariance of the MLE carries over to the multi-parameter case so that $\widehat{g(\boldsymbol{\theta})}$ is the MLE for a (potentially multi-output) function $g(\boldsymbol{\theta})$ of the parameters $\boldsymbol{\theta}$. We also have a corresponding result for the large sample approximation of the sampling distribution of $\widehat{g(\boldsymbol{\theta})}$, which similarly can be derived from a first order Taylor expansion of the function around $\hat{\boldsymbol{\theta}}$.

Theorem 21. *The approximate sampling distribution for the MLE of a multi-output function $g(\boldsymbol{\theta})$ in large samples is*

$$\widehat{g(\boldsymbol{\theta})}(Y_1, \ldots, Y_n) \overset{\text{approx}}{\sim} N\left(g(\boldsymbol{\theta}), g'(\hat{\boldsymbol{\theta}})\mathcal{J}_n^{-1}(\hat{\boldsymbol{\theta}})g'(\hat{\boldsymbol{\theta}})^\top\right),$$

as $n \to \infty$, where

$$g'(\hat{\boldsymbol{\theta}}) = \frac{\partial g(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\Big|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}}$$

is the Jacobian matrix (matrix of all partial derivatives) of the transformation evaluated at the MLE $\hat{\boldsymbol{\theta}}$.

9 Regression

9.1 Linear Gaussian regression

$$Y_i = \boldsymbol{x}_i^\top \boldsymbol{\beta} + \varepsilon_i, \quad \varepsilon_i \overset{\text{iid}}{\sim} N(0, \sigma_\varepsilon^2)$$

$$\begin{aligned} Y_i \mid \boldsymbol{x}_i &\overset{\text{ind}}{\sim} N(\mu_i, \sigma_\varepsilon^2) \\ \mu_i &= \boldsymbol{x}_i^\top \boldsymbol{\beta} \end{aligned} \tag{9.1}$$

9.2 Logistic regression

$$Y_i \mid \boldsymbol{x}_i \overset{\text{ind}}{\sim} \text{Bernoulli}(\mu_i)$$

$$\mu_i = \Pr(Y_i = 1 \mid \boldsymbol{x}_i) = \frac{1}{1 + e^{-\boldsymbol{x}_i^\top \boldsymbol{\beta}}}$$

$$\begin{aligned} Y_i \mid \boldsymbol{x}_i &\overset{\text{ind}}{\sim} \text{Bernoulli}(\mu_i) \\ \mu_i &= \frac{1}{1 + e^{-\boldsymbol{x}_i^\top \boldsymbol{\beta}}} \end{aligned} \tag{9.2}$$

9.3 Poisson regression

$$Y_i \mid \boldsymbol{x}_i \overset{\text{ind}}{\sim} \text{Poisson}(\mu_i)$$

$$\begin{aligned} Y_i \mid \boldsymbol{x}_i &\overset{\text{ind}}{\sim} \text{Poisson}(\mu_i) \\ \mu_i &= e^{\boldsymbol{x}_i^\top \boldsymbol{\beta}} \end{aligned} \tag{9.3}$$

$$\begin{aligned} Y_i \mid \boldsymbol{x}_i &\overset{\text{ind}}{\sim} \text{Negbin}(r, \mu_i) \\ \mu_i &= e^{\boldsymbol{x}_i^\top \boldsymbol{\beta}} \end{aligned} \tag{9.4}$$

9.4 Generalized linear models

$$
\begin{aligned}
Y_i \mid \boldsymbol{x}_i &\overset{\text{ind}}{\sim} \text{Gamma}(\alpha, e^{\boldsymbol{x}_i^\top \boldsymbol{\beta}}) \\
\mu_i &= \alpha e^{\boldsymbol{x}_i^\top \boldsymbol{\beta}}
\end{aligned} \tag{9.5}
$$

9.5 Nonlinear Gaussian regression

Polynomial regression

9.6 Cross-validation

9.7 Regularization

9.8 Interactions and Regression trees

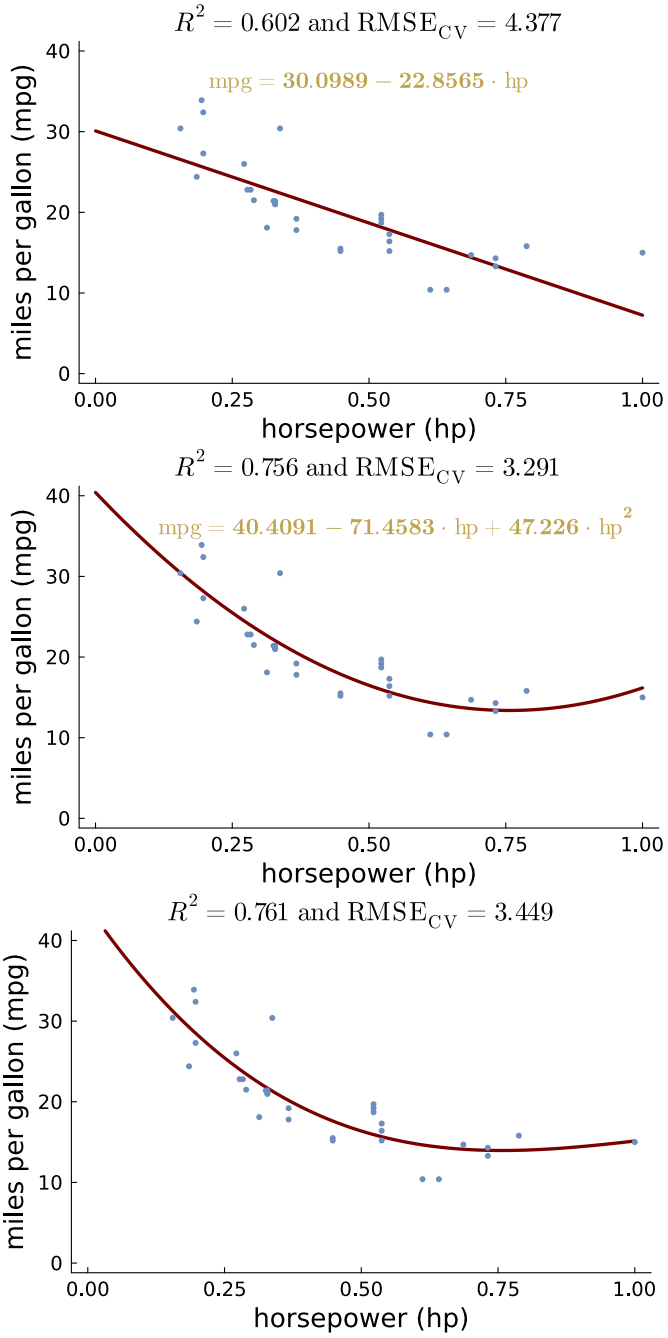

Figure 9.1: Fitting polynomial regression models to the mtcars data.

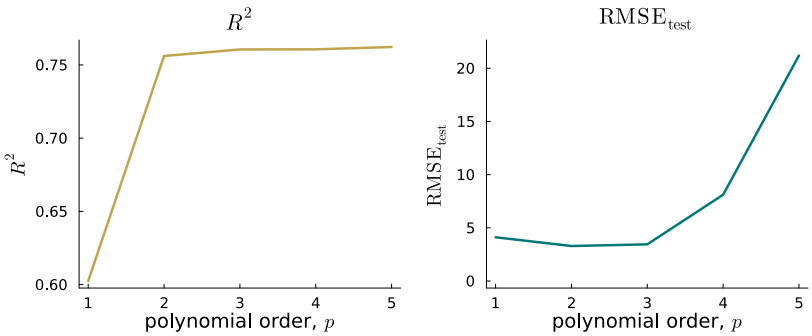

Figure 9.2: In-sample R^2 (left) and cross-validated RMSE (right) when fitting polynomials of different order to the mtcars data.

10 Time series

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Answers to selected exercises

Chapter 1.1, page 12

1. No, since $3/2 = 1.5$ it is not a whole number; it has decimal point.
2. No, it is rational since it can be written as a ratio of integers $1.75 = 7/4$.

Chapter 1.2, page 13

1. $\frac{1}{2} + \frac{3}{4} = \frac{2}{4} + \frac{3}{4} = \frac{5}{4}$
2. $\frac{1}{3} + \frac{3}{4} = \frac{4}{3 \cdot 4} + \frac{3 \cdot 3}{3 \cdot 4} = \frac{4+9}{12} = \frac{13}{12}$
3. $ac - a(b + c) = ac - ab - ac = -ab$
4. $a\left(\frac{a}{b}\right) = \frac{a \cdot a}{b} = \frac{a^2}{b}$
5. $\frac{2}{4} \cdot \frac{3}{2} = \frac{2 \cdot 3}{4 \cdot 2} = \frac{6}{8} = \frac{3}{4}$
6. $2 \cdot 4 + \frac{15}{3 \cdot 5} = 8 + \frac{15}{15} = 8 + 1 = 9$
7. $\frac{\frac{5}{4}}{3} = \frac{\frac{5}{4}}{\frac{3}{1}} = \frac{5 \cdot 1}{4 \cdot 3} = \frac{5}{12}$
8. $a^2 - b^2 + a + b = (a + b)(a - b) + a + b = (a + b)(a - b + 1)$
9. $(a + b)^2 - (a - b)^2 = a^2 + 2ab + b^2 - (a^2 - 2ab + b^2) = 4ab$

Chapter 1.3, page 14

1. $3x - 2 = 0 \iff 3x = 2 \iff x = 2/3$
2. $4x + 3 = 0.5x \iff 4x - 0.5x = -3 \iff 3.5x = -3 \iff x = -3/3.5 = -6/7$
3. $2y + 3x = 4 \iff 2y = 4 - 3x \iff y = 2 - 3/2x$
4. $2 + x \geq 4 \overset{\text{subtract } 2}{\iff} 2 + x - 2 \geq 4 - 2 \iff x \geq 2$
5. $1 - x > -6 \overset{\text{add } -1}{\iff} -x > -6 - 1 = -7 \overset{\text{multiply } -1}{\iff} x < 7$ (multiplication with negative number reverses the inequality).

Chapter 1.4, page 16

1. $\sum_{k=1}^{4} k = 1 + 2 + 3 + 4 = 10$
2. $\sum_{i=1}^{4} k = k + k + k + k = 4k$ (trick question! note that each term

in the sum is the constant k, which is the same in each term as the index variable i ranges from 1 to 4.)

3. $\sum_{y=1}^{3} y^2 = 1^2 + 2^2 + 3^2 = 1 + 4 + 9 = 14$
4. $\left(\sum_{y=1}^{3} y\right)^2 = \left(1 + 2 + 3\right)^2 = 6^2 = 36$
5. $\prod_{k=1}^{4} k = 1 \cdot 2 \cdot 3 \cdot 4 = 24$
6. $\prod_{i=1}^{4} k = k \cdot k \cdot k \cdot k = k^4$ (did you fall for it again?)
7. $\prod_{i=1}^{3} i^2 = 1^2 \cdot 2^2 \cdot 3^2 = 1 \cdot 4 \cdot 9 = 36$
8. $\left(\prod_{i=1}^{3} i\right)^2 = \left(1 \cdot 2 \cdot 3\right)^2 = 6^2 = 36$

Chapter 1.5, page 20

1. There are $4^3 = 64$ different ways that 3 balls can be drawn from an urn with 4 different colored balls, with replacement and with respect to the order in which the balls are drawn.
2. There are $\binom{4}{2} = \frac{4!}{2!(4-2)!} = 6$ different ways that two friends can be selected to join you at the cinema, provided that out only care about which two are joining and not the order in which they are selected.

Chapter 1.6, page 22

1. $(-2)^3 = (-2)(-2)(-2) = 4(-2) = -8$.
2. $0.1^2 = \left(\frac{1}{10}\right)^2 = \frac{1}{10} \cdot \frac{1}{10} = \frac{1}{100} = 0.01$.
3. $3^2 \cdot 3^5 = 9 \cdot 243 = 2187$.
4. $(2^4)^2 = (16)^2 = 256$.
5. $\frac{a^3}{a^2} = a^{3-2} = a^1 = a$.
6. $\frac{a^3}{a^5} = a^{3-5} = a^{-2} = \frac{1}{a^2}$.
7. $\frac{6^3}{2^3} = \left(\frac{6}{2}\right)^3 = 3^3 = 27$.
8. $\frac{6 \cdot 10^{-4}}{3 \cdot 10^{-6}} = 2 \cdot 10^{-4-(-6)} = 2 \cdot 10^2 = 2 \cdot 100 = 200$.
9. Simplify $a \cdot \frac{b^2}{a^3} = \frac{b^2}{a^2} = \left(\frac{b}{a}\right)^2$.

Chapter 1.7, page 24

1. $e^{\ln(3)} = 3$ since the (natural) exponential and logarithm are each other's inverses we have $e^{\ln(a)} = a$ for any a
2. $\ln(e^4 e^{-2}) = \ln(e^{4-2}) = \ln(e^2) = 2$
3. $\frac{6e^{3x}}{2e^x} = 3e^{3x-x} = 3e^{2x}$
4. $\log_2(8) + \log_3(27) = \log_2(2^3) + \log_3(3^3) = 3 + 3 = 6$ since $\log_b(b^x)$ for any base b by the definition of the logarithm.
5. $3^{2x-1} = 27 \Leftrightarrow 3^{2x-1} = 3^3 \Leftrightarrow 2x - 1 = 3 \Leftrightarrow 2x = 4$, with solution $x = 2$
6. $2 - \ln(3x - 2) = 10 \Leftrightarrow \ln(3x - 2) = -8 \Leftrightarrow e^{\ln(3x-2)} = e^{-8} \Leftrightarrow$

$3x - 2 = e^{-8}$ with solution $x = \frac{1}{3}(2 + e^{-8})$

7. $\ln(x) - \ln(x-2) = 2 \Leftrightarrow \ln\left(\frac{x}{x-2}\right) = 2 \Leftrightarrow \frac{x}{x-2} = e^2 \Leftrightarrow$ $x = xe^2 - 2e^2 \Leftrightarrow 2e^2 = x(e^2 - 1)$ with solution $x = \frac{2e^2}{e^2-1}$
8. $y = \ln\left(\frac{x}{1-x}\right) \Leftrightarrow e^y = \frac{x}{1-x}$ with solution $x = \frac{e^y}{1+e^y}$

Chapter 1.8, page 28

1. $f(2) = 2^2 + 3^2 = 4 + 9 = 13$ and $f(-1) = (-1)^2 + 3^(- 1) = 1 + \frac{1}{3}$, so $f(2) - f(-1) = 13 - (1 + \frac{1}{3}) \approx 11.666$
2.

Chapter 1.9, page 30

1. Here is the code in the Julia language:

```
# inner function
function h(x)
  return x^2
end

# outer function
function g(x)
  return log(x)
end

# composite function
function f(x)
  return g(h(x))
end
```

Chapter 1.10, page 31

1. A solution.

Chapter 1.11, page 33

1. A solution.

Chapter 1.12, page 39

1. We get $f(1.1) \approx 2.10000$, $f(1.01) \approx 2.00999$, $f(1.001) \approx 2.00099$ and $f(1.0001) \approx 2.00009$, so it seems that the $f(x)$ settles down at the limiting value of 2 as x approaches 1.
2. We need to see if we can isolate a common factor in the numerator and denominator. We have $f(x) = \frac{x^2-1}{x-1} = \frac{(x-1)(x+1)}{x-1} = x + 1$. So $\lim_{x\to 1} \frac{x^2-1}{x-1} = \lim_{x\to 1}(x + 1) = 1 + 1 = 2$.
3. Diving both numerator and denominator of the function $\frac{2x^2-3x+1}{3x^2+4}$ by x^2 gives

$$\frac{2x^2 - 3x + 1}{3x^2 + 4} = \frac{2 - \frac{3}{x} + \frac{1}{x^2}}{3 + \frac{4}{x^2}}$$

Since all terms that involve x are of the form $\frac{1}{x}$ or $\frac{1}{x^2}$ they all approach zero when $x \to \infty$ and therefore

$$\lim_{x\to\infty} \frac{2x^2 - 3x + 1}{3x^2 + 4} = \lim_{x\to\infty} \frac{2 - \frac{3}{x} + \frac{1}{x^2}}{3 + \frac{4}{x^2}} = \frac{2}{3}$$

Chapter 1.13, page 41

1. It is left-continuous at $x = 0$ since

$$\lim_{x\to 0^-} f(x) = f(0) = 0$$

but not right-continuous at $x = 0$ since

$$\lim_{x\to 0^+} f(x) = 1 \neq f(0) = 0$$

It is therefore not continuous at $x = 0$.

Chapter 1.14, page 53

1. The power rule gives

$$\frac{\mathrm{d}}{\mathrm{d}x} 3x^2 = 2 \cdot 3x = 6x.$$

2. The sum, constant and power rule gives

$$\frac{\mathrm{d}}{\mathrm{d}x}(1 + 3x^2) = 0 + 6x = 6x.$$

3. The sum and power rule gives

$$\frac{\mathrm{d}}{\mathrm{d}x}(3x^2 + 2x) = 6x + 2.$$

4. The chain rule (outer function $g(x) = e^x$ and inner function $h(x) = 2x$) gives

$$\frac{\mathrm{d}}{\mathrm{d}x}(e^{2x}) = e^{2x} \cdot 2 = 2e^{2x}.$$

5.

$$\frac{\mathrm{d}}{\mathrm{d}x}(e^{-3x}) = -3e^{-3x}.$$

6. Since

$$\frac{\mathrm{d}}{\mathrm{d}y}\left(\frac{1}{1+y}\right)^2 = \frac{\mathrm{d}}{\mathrm{d}y}(1+y)^{-2}$$

The chain rule (outer function $g(x) = x^{-2}$ and inner function $h(x) = 1 + y$) gives

$$\frac{\mathrm{d}}{\mathrm{d}y}(1+y)^{-2} = -2(1+y)^{-3} \cdot \frac{\mathrm{d}}{\mathrm{d}y}(1+y) = -2\Big(\frac{1}{1+y}\Big)^3.$$

7. The product rule gives

$$\frac{\mathrm{d}}{\mathrm{d}x}(x^2e^x) = 2xe^x + x^2e^x = e^x(2x + x^2) = e^x x(2 + x).$$

8. The quotient rule gives

$$\frac{\mathrm{d}}{\mathrm{d}x}(\frac{x^2}{e^x}) = \frac{2xe^x - x^2e^x}{(e^x)^2} = \frac{e^x(x(2-x))}{e^{2x}} = \frac{x(2-x)}{e^x}.$$

9. The product and power rule gives

$$\frac{\mathrm{d}}{\mathrm{d}x}(x^{-2}e^x) = (-2)x^{-3}e^x + x^{-2}e^x = e^x x^{-3}(x-2) = \frac{e^x(x-2)}{x^3}.$$

10. The first derivative is

$$f'(x) = \frac{\mathrm{d}}{\mathrm{d}x}(x^3 + 2x^2 + 4) = 3x^2 + 4x$$

The second derivative is

$$f''(x) = \frac{\mathrm{d}}{\mathrm{d}x}f'(x) = \frac{\mathrm{d}}{\mathrm{d}x}(3x^2 + 4x) = 6x + 4$$

11. The first derivative is

$$f'(x) = \frac{\mathrm{d}}{\mathrm{d}x}(\exp(x)) = \exp(x)$$

The second derivative is

$$f''(x) = \frac{\mathrm{d}}{\mathrm{d}x}f'(x) = \frac{\mathrm{d}}{\mathrm{d}x}(\exp(x)) = \exp(x)$$

12. The first derivative is

$$f'(x) = \frac{\mathrm{d}}{\mathrm{d}x}(\ln(x)) = \frac{1}{x}$$

The second derivative is

$$f''(x) = \frac{\mathrm{d}}{\mathrm{d}x}f'(x) = \frac{\mathrm{d}}{\mathrm{d}x}\Big(\frac{1}{x}\Big) = -\frac{1}{x^2}$$

13. The first derivative of the square function being $f'(x) = 2x$ means that the slope of the tangent line goes from a negative value to positive value as x travels from negative to positive values. The second derivative is $f''(x) = 2$ is a postitive constant for all x because the square function is accelerating upwards at a constant rate across all x.
14. The partial derivative with respect to x is

$$f_x(x,y) = \frac{\partial}{\partial x}(x^3 y) = 3x^2 y$$

The partial derivative with respect to y is

$$f_y(x,y) = \frac{\partial}{\partial y}(x^3 y) = x^3$$

15. The partial derivative with respect to x is

$$f_x(x,y) = \frac{\partial}{\partial x}(\exp(xy)) = y\exp(xy)$$

The partial derivative with respect to y is

$$f_y(x,y) = \frac{\partial}{\partial y}(\exp(xy)) = x\exp(xy)$$

16. The partial derivative with respect to x is

$$f_x(x,y) = \frac{\partial}{\partial x}(x^2 \log(y) e^y) = 2x\log(y)e^y$$

The partial derivative with respect to y is

$$f_y(x,y) = \frac{\partial}{\partial y}(x^2 \log(y) e^y) = x^2\Big(\frac{1}{y}e^y + \log(y)e^y\Big)$$

17. Since $f_x(x,y) = \frac{\partial}{\partial x}(x + xy^2) = 1 + y^2$ we have the second partial derivative with respect to x as

$$f_{xx}(x,y) = \frac{\partial}{\partial x}(1 + y^2) = 0.$$

Since $f_y(x,y) = \frac{\partial}{\partial y}(x + xy^2) = 2xy$ we have the second partial derivative with respect to y as

$$f_{yy}(x,y) = \frac{\partial}{\partial y}(2xy) = 2x.$$

and the cross partial derivative

$$f_{xy}(x,y) = \frac{\partial}{\partial y} f_x(x,y) = \frac{\partial}{\partial y}(1 + y^2) = 2y$$

Chapter 1.15, page 67

1. answer here later

Chapter 1.16, page 79

1. $\int_1^2 3(x+1)^2\,\mathrm{d}x = [(x+1)^3]_1^2 = (2+1)^3 - (1+1)^3 = 27 - 8 = 19$
2. Compute the definite integral $\int_1^2 e^x\,\mathrm{d}x = [e^x]_1^2 = e^2 - e^1 = e(e-1) \approx 4.6707$
3. $\int_0^5 3\,\mathrm{d}x = [3x]_0^5 = 3\cdot 5 - 3\cdot 0 = 15$
4. $$\int_0^3 (1.5t^2 + t)\,\mathrm{d}t = [0.5t^3 + 0.5t^2]_0^3 = 0.5\cdot 3^3 + 0.5\cdot 3^2 = 18$$
5. $$\int \frac{1}{y^5}\,\mathrm{d}y = -\frac{1}{4y^4} + C$$
6. $$\int y(\frac{3}{2}y^2 + y)\,\mathrm{d}y = \frac{3}{8}y^4 + \frac{1}{3}y^3 + C$$
7. $$\int_{y_1=0}^{y_1=2} e^{-y_1}\,\mathrm{d}y_1 = [-e^{-y_1}]_0^2 = -e^{-2} - (e^{-0}) = 1 - e^{-2}$$
8. $$\int_{y_1=0}^{y_1=2} e^{-y_2}\,\mathrm{d}y_1 = e^{-y_2}[y_1]_0^2 = 2e^{-y_2}$$
9. This is an improper integral since the upper limit of integration is infinity. We can compute the integral using the two-step approach described in the text:

$$\begin{aligned}
\int_0^\infty \frac{1}{2}e^{-x/2}\,\mathrm{d}x &= \lim_{b\to\infty}\int_0^b \frac{1}{2}e^{-x/2}\,\mathrm{d}x && (1.11)\\
&= \lim_{b\to\infty}[-e^{-x/2}]_0^b && (1.12)\\
&= \lim_{b\to\infty}\left(-e^{-b/2} - (-1)\right) && (1.13)\\
&= \lim_{b\to\infty}\left(-e^{-b/2}\right) + 1 = 1 && (1.14)
\end{aligned}$$

Chapter 1.17, page 82

1. Answer here.

Chapter 1.18, page 92

1. Answer here.

Chapter 6.1, page 156

1. The cdf of X is given by

$$F_X(x) = \int_0^x f_X(t)dt = \int_0^x \frac{t}{2}dt = \frac{1}{2} \cdot \frac{x^2}{2} = \frac{x^2}{4}, \text{ for } 0 < x < 2.$$

Hence the cdf of Y is

$$F_Y(y) = \Pr(Y \leq y) = \Pr(\exp(X) \leq y) = \Pr(X \leq \log(y)) = F_X\Big(\log(y)\Big)$$
$$= \Big(\frac{\log(y)}{4}\Big)^2, \text{ for } 1 < y < e^2.$$

The pdf of Y is given by

$$f_Y(y) = \frac{\mathrm{d}}{\mathrm{d}y}F_Y(y) = \frac{\mathrm{d}}{\mathrm{d}y}\Big(\frac{\log(y)}{4}\Big)^2 = \frac{1}{4} \cdot 2 \cdot \frac{1}{y} = \frac{1}{2y}, \text{ for } 1 < y < e^2.$$

2. The transformation formula can be used directly since the transformation is monotone. The inverse function $x = g^{-1}(y)$ is obtained by solving the equation $y = -\beta\log(x)$ for x. Dividing both sides with $-\beta$ and then exponentiating both sides (remember $\exp(\log(x)) = x$) we get

$$g^{-1}(y) = \exp\Big(-\frac{y}{\beta}\Big),$$

with derivative (using the chain rule)

$$\frac{\mathrm{d}}{\mathrm{d}y}g^{-1}(y) = -\frac{1}{\beta}\exp\Big(-\frac{y}{\beta}\Big).$$

Hence, the pdf of Y is according to the transformation formula

$$f_Y(y) = f_X\Big(g^{-1}(y)\Big)\left|\frac{\mathrm{d}}{\mathrm{d}y}g^{-1}(y)\right|$$
$$= f_X\Big(\exp(-\frac{y}{\beta})\Big) \cdot \frac{1}{\beta}\exp(-\frac{y}{\beta})$$
$$= 1 \cdot \frac{1}{\beta}\exp(-\frac{y}{\beta}) = \frac{1}{\beta}\exp(-\frac{y}{\beta}).$$

Note that since the pdf for the uniform is just $f_X(x) = 1$ over the support $0 \leq x \leq 1$, i.e. the density is not a function of x, it looks a little weird when we plug in the inverse function $g^{-1}(y)$ into the pdf, since the end result is still 1. Since the support of X is $0 \leq x \leq 1$, the support for the transformed variable is $0 < y < \infty$. We recognize this as the pdf of an *exponential distribution* with scale parameter β.

3. The transformation is again monotone and we can use the transformation formula. The inverse function is $x = g^{-1}(y) = \frac{e^y}{1+e^y}$, with derivative

$$\frac{\mathrm{d}}{\mathrm{d}y} g^{-1}(y) = \frac{e^y}{(1+e^y)^2}.$$

The pdf of $X \sim \text{Beta}(\alpha, \beta)$ is

$$f_X(x) = \frac{1}{B(\alpha,\beta)} x^{\alpha-1}(1-x)^{\beta-1}, \text{ for } 0 < x < 1,$$

where $B(\alpha, \beta)$ is the beta function. The pdf of Y is then

$$\begin{aligned} f_Y(y) &= f_X\Big(g^{-1}(y)\Big) \left| \frac{\mathrm{d}}{\mathrm{d}y} g^{-1}(y) \right| \\ &= f_X\Big(\frac{e^y}{1+e^y}\Big) \cdot \frac{e^y}{(1+e^y)^2} \\ &= \frac{1}{B(\alpha,\beta)} \left(\frac{e^y}{1+e^y}\right)^{\alpha-1} \left(1 - \frac{e^y}{1+e^y}\right)^{\beta-1} \cdot \frac{e^y}{(1+e^y)^2} \\ &= \frac{1}{B(\alpha,\beta)} \left(\frac{e^y}{1+e^y}\right)^{\alpha-1} \left(\frac{1}{1+e^y}\right)^{\beta-1} \cdot \frac{e^y}{(1+e^y)^2} \\ &= \frac{1}{B(\alpha,\beta)} \cdot \frac{e^{\alpha y}}{(1+e^y)^{\alpha+\beta}} \end{aligned}$$

The support of Y is $-\infty < y < \infty$. This is the pdf of a *logistic-beta distribution* with parameters α and β. It is also called the Z-distribution. See this observable widget.

Chapter 7.1, page 177

1. Since a joint density must integrate to one over the whole support, we can determine c from the equation

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x,y)\,\mathrm{d}y\,\mathrm{d}x = \int_0^1 \int_0^1 cx^2\,\mathrm{d}y\,\mathrm{d}x = 1.$$

We have

$$\begin{aligned} \int_0^1 \int_0^1 cx^2\,\mathrm{d}y\,\mathrm{d}x &= \int_0^1 cx^2\,[y]_0^1\,\mathrm{d}x = c\int_0^1 x^2\,\mathrm{d}x \\ &= c\left[\frac{x^3}{3}\right]_0^1 = \frac{c}{3}. \end{aligned}$$

Hence, $\frac{c}{3} = 1$ whith the solution $c = 3$.

2. The function is non-negative $f(x,y) \geq 0$ for all $0 < x < 1$ and $0 < y < x$, and we have

$$\begin{aligned} \int_0^1 \int_0^x 10x^2 y\,\mathrm{d}y\,\mathrm{d}x &= \int_0^1 10x^2 \left[\frac{y^2}{2}\right]_0^x \mathrm{d}x = \int_0^1 10x^2 \cdot \frac{x^2}{2}\,\mathrm{d}x \\ &= 5\int_0^1 x^4\,\mathrm{d}x = 5\left[\frac{x^5}{5}\right]_0^1 = 1. \end{aligned}$$

Hence, the function is a valid joint density function.

Chapter 8.1, page 183

1. The likelihood from an iid sample from Expon(θ) is

$$p(x_1, \ldots, x_n|\theta) = \prod_{i=1}^{n} p(x_i|\theta) = \prod_{i=1}^{n} \theta e^{-\theta x_i} = \theta^n e^{-\theta \sum_{i=1}^{n} x_i}$$

The log-likelihood is therefore

$$\ell(\theta) = n \log(\theta) - \theta \sum_{i=1}^{n} x_i$$

Setting the first derivative to zero

$$\frac{\mathrm{d}}{\mathrm{d}\theta} \ell(\theta) = \frac{n}{\theta} - \sum_{i=1}^{n} x_i = 0$$

and solving for θ gives the maximum likelihood estimator

$$\hat{\theta} = \frac{n}{\sum_{i=1}^{n} x_i} = \frac{1}{\bar{x}},$$

where $\bar{x} = n^{-1} \sum_{i=1}^{n} x_i$ is the sample mean. To verify that this is indeed a maximum, we check the second derivative at the (supposedly) maximum likelihood estimate

$$\frac{\mathrm{d}^2}{\mathrm{d}\theta^2} \ell(\theta)|_{\theta=\hat{\theta}} = -\frac{n}{\hat{\theta}^2} = -\frac{n}{\left(\frac{1}{\bar{x}}\right)^2} = -n\bar{x}^2 < 0.$$

Since the second derivative is zero at $\hat{\theta} = \frac{1}{\bar{x}}$, this indeed a maximizer.

2. Let $\mathcal{U}$ denote the set of observation indices for the observed, uncensored, observations and let $\mathcal{C}$ denote the observation indices for the censored observations. The likelihood for all data, censored and uncensored, is then

$$p(x_1, \ldots, x_n|\theta) = \prod_{i=1}^{n} p(x_i|\theta) \tag{8.19}$$

$$= \prod_{u \in \mathcal{U}} p(x_u|\theta) \prod_{c \in \mathcal{C}} p(x_c|\theta) \tag{8.20}$$

For the uth observed observation, the contribution to the likelihood is $p(x_u|\theta) = \theta e^{-\theta x_u}$, which is the exponential density evaluated at the observed x_u. So the part of the likelihood coming from the observed data is the same as in previous exercise

$$\prod_{u \in \mathcal{U}} p(x_u|\theta) = \prod_{u \in \mathcal{U}} \theta e^{-\theta x_u} = \theta^{n_u} e^{-\theta \sum_{u \in \mathcal{U}} x_u},$$

For the censored observations we only know that their values are *at least as large* as the value at the end of the study x_c; hence, the cth censored observation contributes the term

$$\Pr(X \geq x_c) = 1 - F(x_c|\theta),$$

where $F(x_c|\theta) = 1 - e^{-x_c\theta}$ is the distribution function for an exponential variable X_c with parameter θ. So, the likelihood for all observations is

$$\begin{aligned} p(x_1, \ldots, x_n|\theta) &= \prod_{u\in\mathcal{U}} p(x_u|\theta) \prod_{c\in\mathcal{C}} (1 - F(x_c|\theta)) && (8.21)\\ &= \theta^{n_u} e^{-\theta\sum_{u\in\mathcal{U}} x_u} \times e^{-\theta\sum_{u\in\mathcal{U}} x_c} && (8.22)\\ &= \theta^{n_u} e^{-\theta\sum_{i=1}^{n} x_i}, && (8.23) \end{aligned}$$

which is nearly of the same form as for the case when there was no censoring; the only difference is that the power of θ in the first factor is now n_u, the number of uncensored observations, not the total number of observations $n = n_u + n_c$. The maximum likelihood estimator is obtained as in the previous exercise by solving for θ in

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\ell(\theta) = \frac{n_u}{\theta} - \sum_{i=1}^{n} x_i = 0,$$

which gives the maximum likelihood estimator $\hat{\theta} = \frac{n_u}{\sum_{i=1}^{n} x_i}$.

Chapter 8.2, page 185

1. We first need to compute the second derivative of the log-likelihood function. The log-likelihood function is

$$\ell(p) = \sum_{i=1}^{n} \Big(x_i \log p + (1 - x_i) \log(1 - p) \Big) = s \log p + f \log(1 - p)$$

where $s = \sum_{i=1}^{n} x_i$ is the number of successes in the sample, and $f = n - s$ is the number of failures. The first derivative (using the chain rule) is

$$\frac{\mathrm{d}}{\mathrm{d}p}\ell(p) = \frac{s}{p} - \frac{f}{1 - p}$$

Setting the first derivative to zero, and solving for p, gives the MLE $\hat{p} = s/n$. The second derivative is

$$\frac{\mathrm{d}^2}{\mathrm{d}p^2}\ell(p) = -\frac{s}{p^2} - \frac{f}{(1 - p)^2}$$

The observed information is therefore

$$\begin{aligned} \mathcal{J}_n(\hat{p}) = -\ell''(\hat{p}) &= \frac{s}{\hat{p}^2} + \frac{f}{(1 - \hat{p})^2} = \frac{s}{(s/n)^2} + \frac{f}{(f/n)^2}\\ &= \frac{n}{s/n} + \frac{n}{f/n} = \frac{n}{\hat{p}(1 - \hat{p})}. \end{aligned}$$

The Fisher information is

$$\mathcal{I}_n(p) = \mathbb{E}\left(-\ell''(p)\right) = \mathbb{E}\left(\frac{s}{p^2} + \frac{f}{(1-p)^2}\right) = \left(\frac{\mathbb{E}(s)}{p^2} + \frac{\mathbb{E}(f)}{(1-p)^2}\right)$$
$$= \frac{np}{p^2} + \frac{n(1-p)}{(1-p)^2} = \frac{n}{p} + \frac{n}{(1-p)} = \frac{n}{p(1-p)},$$

since $\mathbb{E}(s) = np$ and $\mathbb{E}(f) = n(1-p)$ from the Binomial distribution.

2. TBD

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