Foundations of Statistics

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Contents

Preliminaries

Overview

In this course the fundamental principles and techniques underlying modern statistical and data analysis will be introduced. The course will cover the core foundations of statistical theory consisting of:

- probability distributions and techniques;
- statistical concepts and methods;
- linear models.

The course highlights the importance of computers, and in particular, statistical packages, in performing modern statistical analysis. Students will be introduced to the statistical package **R** as a statistical and programming tool and will gain experience in interpreting and communicating its output.

Learning Outcomes

A student who completes this module successfully will be able to:

- derive and explain properties of basic statistical inference; linear regression models and probability techniques;
- perform exploratory data analysis; summarising their analysis and proposing further investigations;
- derive point and interval estimators, and perform hypothesis tests for a variety of situations;
- apply the theory and methods for statistical inference, linear regression models and probability techniques to a wide range of practical examples;
- use the statistical package **R** to derive results concerning statistical inference;

- communicate their statistical analysis in a written report.

Syllabus Overview

- Summary statistics and visualising data
- Probability, random variables and expectation
- Joint distributions, conditional distribution, covariance and correlation
- Central limit theorem
- Parameter estimation - Method of Moments and Maximum Likelihood Estimation
- Transformations of random variables
- Multivariate normal distribution
- Linear Models
- Least squares estimation
- Interval estimation
- Hypothesis testing and goodness-of-fit
- ANOVA

Tasks

At the end of most chapters there are tasks to complete. These tasks will either be computer lab sessions using the statistical package **R** or statistical exercises or both to reinforce the material covered in the chapter (or the last couple of chapters).

Chapter 1

Introduction

1.1 What is Statistics?

Watch Video 1: What is Statistics?

Statistics is the field of mathematics concerned with reasoning about data and uncertainty.

This includes collecting, organising, summarising, analysing and presenting data.

In particular, Statistics provides the tools for making decisions and drawing conclusions from data in a principled way—this is called **statistical inference**.

A key part of statistics is **communicating**: communicating context, data, assumptions, analysis, results.

1.2 Populations and samples

A key idea in Statistics is to draw conclusions about a **population** based on a **sample** from that population. This is where the word *inference* comes from: we are *inferring* something about the population based on the sample.

Population
A **population** is a group or collection of similar individuals (*e.g. students*), items (*e.g. plants*) or events (*e.g. days*) that are of interest to us.

When we want to make inferences about a population, it would be very time consuming and expensive to look at every member of the population. It could also be destructive if the experiment involves testing until failure.

Sample
A **sample** is a subset of the population.

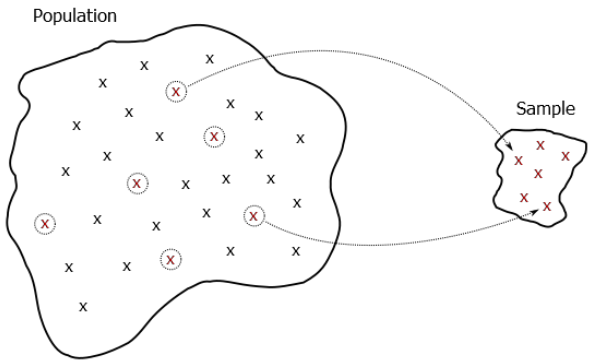


Figure 1.1: A sample is a subset of the population. Each x here represents a sampling unit; red shows the ones in the sample.

Example 1.2.1.
Population: The students studying mathematics.
Sample A: Those students who were born in London.
Sample B: Female students.

Example 1.2.2.
Population: Female students at University of Nottingham.
Sample A: Ten randomly chosen female students.
Sample B: Ten randomly chosen female students from mathematics.

If inferences about the population based on sample data are to make sense, **the sample must be representative** of the population.

In Example 1.2.1, neither Sample A nor Sample B are very representative of the population. Suppose, say, we wanted to infer the proportion of all students on this module that are over 1.8m tall: why would basing the inference on a sample of only females be a bad idea?

In Example 1.2.2, these samples are **random samples**. Random sampling is often used to help ensure the sample is representative of population.

The individual items in the population and sample are called **elements** or **sampling units**. In conducting an experiment we are trying to learn about particular aspects or phenomena of the population of elements. These unknown phenomena are known as **random variables** and in an experiment we observe a random variable on each element in the sample in order to make inferences about the values of the random variable in the population.

Often the population is large enough compared to the sample size to be assumed **infinite**; e.g., the population of the UK is much greater than a sample of 100

taken from that population.

Example 1.2.3.
Population: Everyone in the UK.
Random variable: Height.
Take a random sample of people and measure their height.

Example 1.2.4.
Population: Litters of one breed of dog.
Random variable: Number of puppies in a litter.
Take a random sample of litters and count the number of puppies in each litter.

1.3 Types of Data

A measurement of a random variable is commonly termed an **observation** and a collection of observations is called **data**. The set of outcomes that an observation can take is called the **sample space** and we formalise this in Section 4.3 when we introduce probability.

There are many different types of data. There are two main types of data, numerical (quantitative) and categorical (qualitative) data:

Numerical data
Discrete
Numerical values taking a discrete (usually integer) set of values. (Finite or infinite number of possibilities.)
Example: How many siblings do you have?
Continuous
Numerical values taking values on a continuous range. (Finite or infinite range.)
Example: What is your height in cm?

and

Categorical data
Nominal
Set of values that don't possess a natural ordering.
Example: What is your eye colour?
Ordinal
Set of values that do possess a natural ordering.
Example: Letter grades for assessment.
Binary
Only two possible outcomes.
Example: Do you have a brother?

Enter your data into the Microsoft form. This data will be used anonymously (with data from another course) at various stages in the module. Think about the type of data generated for each question.

Data: Microsoft Form

1.4 Some example datasets

Three data sets we'll use in the Section 2 are as follows.

Cavendish experiment
In 1798, Henry Cavendish conducted an experiment to estimate the density of the earth. His 29 measurements, presented as a multiple of the density of water were:

5.50	5.57	5.42	5.61	5.53	5.47	3.88	5.62	5.63	5.07
5.29	5.34	5.26	5.44	5.46	5.55	5.34	5.30	5.36	5.79
5.75	5.29	5.10	5.86	5.58	5.27	5.85	5.65	5.39	

Coursework marks
The marks of 18 students on a piece of coursework are:

Mark	34	42	44	46	48	50
Frequency	1	2	3	6	3	3

Optometry data
Optometry measurements of eye pressure (IOP/$mmHg$) taken by 40 students. 20 Optometry students and 20 engineering students.

Optometry students

14	15	15	14	15	15	15	14
15	16	15	15	16	15	15	15
15	16	15	15				

Engineering students

16	15	17	19	15	17	13	13
13	23	10	13	20	18	16	12
10	17	8	15				

1.5 Statistical Computing

Throughout this module, and indeed the MSc programme, we will be supporting the statistical theory and methodology with applications using the statistical package **R**. Whilst it is important to understand the theory behinds statistical methods it is very rare to implement statistical methods *by hand* and **R** or another statistical package is used. The old computing adage GIGO (garbage in, garbage out) is relevant to statistical computing. If we tell **R** to do something such as perform a calculation, fit a model or predict future observations, it probably will, but we need to be able to check that the question asked, and the answer given, make sense.

1.6 The statistical paradigm

We have introduced data types and the concept of obtaining a sample from a population. We are now in position to outline the steps involved in statistical analysis from the identification of the population and research question of interest through the statistical analysis to interpretation and communication of the analysis.

Statistical analysis consists of a number of steps:

- Specification of population
- Identification of research question
- Sampling design of a protocol
- Data collection
- Exploratory analysis
- Model specification
- Diagnostics (Model verification)
- Inference
- Interpretation
- Communication

The procedure is not usually linear - some iteration may be necessary.

In the following Sections we discuss ways to summarise (Section 2) and visualise (Section 3) our data before we introduce probability (Section 4) which underpins the mathematical modelling and analysis of data.

Task: Session 1

In Section 23, an introduction to the statistical package **R** is given. This includes downloading **R** and getting started.

Work through Section 23, especially if you are unfamiliar with **R**, and then attempt:
Session 1: Introduction to R

Chapter 2

Summary Statistics

A **statistic** is the generic name given to any quantity calculated from the data. A statistic is therefore a *function* of the data.

We use a **summary statistic** to measure and summarise some aspect of the data. Many simple summary statistics can be divided as one of two types: measures of **location** (Section 2.1), and measures of **spread** (Section 2.2). In Section 2.3 we consider the robustness of summary statistics.

A measure of **location** is *a value "typical" of the data.* Examples include the **mean**, **mode** and **median**.

A measure of **spread** quantifies *how variable the data are.* Examples include the **variance**, **standard deviation**, **range** and **interquartile range**.

2.1 Measures of location

A statistic that is a measure of location summarises the data by giving a single number that is, in some sense, typical of that set of data. There are three commonly used measures of location, of which the **mean** is the most important.

1. **Mean** Suppose that n measurements have been taken on the random variable under investigation, and these are denoted by $x_1, x_2, \ldots, x_n$. The (arithmetic) mean of the observations is usually denoted by $\bar{x}$ and is given by

$$\bar{x} = \frac{x_1 + x_2 + \cdots + x_n}{n} = \frac{1}{n}\sum_{i=1}^{n} x_i. \tag{2.1}$$

   In everyday language we say that $\bar{x}$ is the **average** of the observations.

If data are discrete they are often tabulated as in the Coursework dataset. This makes calculating the mean a little easier. Suppose that f_j denotes the number of times that the number j appears in our data set, then we can write

$$\bar{x} = \sum_{j=1}^{\infty} j \frac{f_j}{n}. \tag{2.2}$$

For an explanation of (2.2) and derivation of the mean of the optometry students data, see Video 2.

Watch Video 2: Derivation of the mean

Sometimes continuous data are grouped into a frequency table — this loses the values of the individual and essentially converts the continuous data to discrete data. The sample mean in this case be estimated by assuming that all the observations in a class interval fall at the mid-point of the interval. Therefore, if we have k intervals with mid-points m_1, m_2, ..., m_k and frequencies $f_1, f_2, \ldots, f_k$ then we treat the mid-points as though they are the discrete data values and we can use the formula in (2.2). When determining the midpoint of an interval, due notice should be taken of any rounding of the individual observations.

2. **Median.** The sample median is defined as the observation with cumulative frequency of $n/2$. This is sometimes used instead of the mean, particularly when the histogram of the observations looks *asymmetric*. The median is obtained by sorting the observations in ascending order and then picking out the middle observation or, equivalently, the $\frac{(n+1)}{2}$th observation. If there are an even number of observations in the sample then the median is taken as the average of the $\frac{n}{2}$th and $(\frac{n}{2}+1)$th observations. The ranking can be done using a stem-and-leaf plot.

Hence the median is the 'middle value' in the sample with half the observations numerically greater than the median and the other half smaller than the median. The mathematical properties of the median are less easy to determine than those of the mean and so the mean is preferred for use in most formal statistical analyses. However, the median is quick to calculate in small samples and is useful in descriptive work.

3. **Mode.** This is the value of the random variable which occurs with greatest frequency. The sample mode for discrete data can be found easily by inspection of the data or by a quick look at a frequency table. It is not realistic to define the sample mode for continuous data (we will see why when introducing continuous probability distributions in Section 5). However when such data have been classified into intervals or categories we can find the **modal class** — the class or interval containing the most number of observations.

2.2 Measures of spread

Given the location of the data, we next need to know whether the observations are concentrated around this value, or dispersed over a much wider range of values. Measures of spread express this idea numerically.

1. **Variance.** The sample variance of n observations, $x_1, x_2, \ldots, x_n$, is usually denoted s^2 and defined as

$$\begin{aligned} s^2 &= \frac{(x_1-\bar{x})^2 + (x_2-\bar{x})^2 + \cdots + (x_n-\bar{x})^2}{n-1} \\ &= \frac{1}{n-1}\sum_{i=1}^{n}(x_i-\bar{x})^2. \end{aligned} \tag{2.3}$$

   It is an average squared distance of the observations from their sample mean value. The adjustment is that the divisor is $(n-1)$ rather than n to correct for a bias (we'll come back to this later in Section 9.3) which occurs because we are measuring from the mean of the data rather than the true mean of the population. It is worth pointing out that the difference between using n and $(n-1)$ is especially important for small samples. This formula can be rearranged to the alternative form

$$s^2 = \frac{1}{n-1}\left(\sum_{i=1}^{n} x_i^2 - n\bar{x}^2\right) = \frac{1}{n-1}\left\{\sum_{i=1}^{n} x_i^2 - \frac{1}{n}\left(\sum_{i=1}^{n} x_i\right)^2\right\} \quad , \tag{2.4}$$

   which initially looks more complicated but is actually simpler calculate: compute first the sums $\sum_i x_i$ and $\sum_i x_i^2$ then the rest is easy.

The alternative form is easy to derive as shown in Video 3. However, before you watch the video, try to derive the result yourself.

Watch Video 3: Derivation of the variance

2. **Standard deviation.** The standard deviation, typically denoted s, is just the positive square root of the variance s^2. It is therefore the root-mean-square deviation of the observations about their sample mean. The standard deviation is in the same units as the original measurements and for this reason it is preferred to the variance as a descriptive measure. However, it is often easier from a theoretical and computational point of view to work with variances. Thus the two measures are complementary.

3. **Range.** This is simply the difference between the largest and smallest observation. It can be very useful for comparing the variability in samples of equal size but it is unfortunately affected by the number of observations; the range usually increases as the number of observations in the data set increases.

4. **Inter-quartile range (IQR).** The quartiles are chosen so that 25% of the data lies below the lower quartile (Q_1) and 25% above the upper quartile (Q_3). Thus the lower quartile, median and upper quartile split the data into four equal portions.

Min	25%	Q_1	25%	Q_2	25%	Q_3	25%	Max

   After the data are arranged in ascending order, the lower quartile is calculated as the $\frac{(n+1)}{4}$th observation and the upper quartile is calculated as the $\frac{3(n+1)}{4}$th observation. When $n+1$ is not divisible by 4 then the quartiles are calculated by performing some simple interpolation rule (see Example 1). The difference between the lower and upper quartiles is called the **interquartile range** and it measures the range of the central 50% of the sample.

Example 2.1. **Quartiles and IQR for Cavendish's data.**

Here $n = 29$, so Q_1 is the '7.5th' observation. The 7th observation is 5.29 and the 8th observation is 5.30, so $Q_1 = 5.295$.

Similarly, Q_3 is the '22.5th' observation. The 22nd observation is 5.61 and the 23rd observation 5.62, so $Q_3 = 5.615$.

The IQR is $5.615 - 5.295 = 0.320$.

Link to Cavendish dataset.

2.3 Robustness of summary statistics

In many circumstances (for example, when the distribution of observations is unimodal and roughly symmetric/unskewed and no outliers exist–see definitions in Section 3–visualisation of data) then the mean, median and mode will be very close together. However, if for example the distribution is very skewed there may be a considerable differences between the three measures. The median is often considered as a better description of location for asymmetric distributions than the mean and is much more **robust** to outliers. In other words, the value of the mean is sensitive to the values of very large or very small observations, whereas the median is not. An amended version of the mean, define to be more robust, is the **trimmed mean**.

The **(α%)-trimmed mean** is computed by deleting the α% smallest observations and the α% largest observations before calculating the mean of what is remaining. Trimmed means are used in many judge based scoring systems such as diving and figure skating.

This is more robust than the mean, but the choice of α is somewhat arbitrary and for this reason the median is usually preferred.

Example 2.3.1. **Robustness.**

Let's calculate the *mean*, *median* and *10%-trimmed mean* for the following data:

$$14, 19, 13, 10, 18, 20, 15, 16, 11, 100$$

The mean = 23.6, and median = $(15 + 16)/2 = 15.5$. Notice how the value 100 seems to be an outlier and that this has affected the mean, which is no longer very representative of the "location" of the data.

For the trimmed mean, we delete the bottom and top 10% of observations and compute the mean of what's left, i.e., we delete 10 and 100, then we get that:

$$\text{The trimmed mean} = (14 + 19 + 13 + 18 + 20 + 15 + 16 + 11)/8 = 15.75$$

So by "trimming" we've gotten rid of the influence of the outlier 100, and the trimmed mean seems a better measure of location compared with the mean.

The *median is robust to outliers*, whereas the mean is not. In Video 4 we demonstrate this using the Cavendish dataset. There is also a link provided to the **R Shiny** app used in the video so that you can explore the data and trimming for yourself.

Watch Video 4: Robust Measures

R Shiny app: Cavendish dataset

We talk about robustness not only for measures of location but also, for example, for measures of spread.

The interquartile range is very robust to outliers, whereas the standard deviation is very sensitive to outliers.

Chapter 3

Visualising data

3.1 Introduction

We have seen different ways of creating numerical summaries:

- Measures of location: Mean, median, mode.
- Measures of spread: Variance, standard deviation, interquartile range.

A numerical summary is useful but a single number (or a few numbers) can only tell us so much about the data.

Studying the data values if there are hundreds or thousands of observations is going to be hard to take in.

Therefore, "if a picture paints a thousand words" then **"a plot captures a thousand data points"!**

In this chapter we'll start by talking about some data features to look out for, then some particular types of plots. In Section 3.2, we discuss basic features of the data such as multimodality, symmetry and outliers. In Section 3.3, we present a wide range of different graphical ways of presenting data and we summarise the pros and cons of the different methods in a summary. Finally, in Section 3.4, we draw together the considerations in summarising and visualising data.

3.2 Some data features

In describing either the way in which observations in a sample are dispersed, or the features of a random variable, we talk about the **distribution** of the observations or random variable.

The observations are our **sample** of data, whereas the random variable represents the **population** from which the data are drawn.

It is important at this stage to distinguish between describing the sample of data and making inferences about the population from which the data are drawn. Plotting the data and obtaining numerical summaries for the data should give some idea of the equivalent features in the population, provided the sample size is large enough.

Hence when describing features in plots, the description should pick out features of the data itself but it should also include inferences about the population distribution the data are drawn from. If the sample size is very small then we may comment that few or no inferences can be made. When displaying data graphically we can see not only where the data are located and how they are dispersed but also the general shape of the distribution and if there are any interesting features.

3.2.1 Multimodal distributions

We also use the word **mode** to describe where a distribution has a *local* maximum. Then we can call a distribution unimodal (one peak), bimodal (two peaks) or multimodal (multiple peaks), e.g. as shown in Figure 3.1.

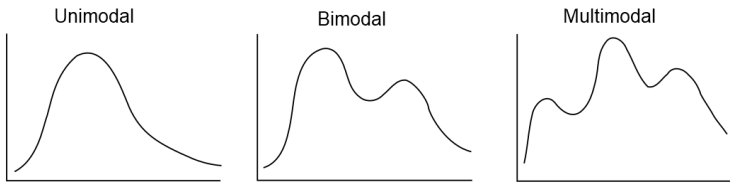


Figure 3.1: Distributions with different numbers of modes.

Sometimes there are gaps in the data, like in Figure 3.2

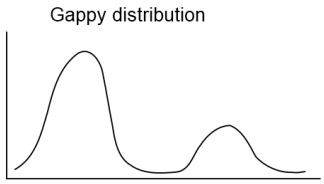


Figure 3.2: A bimodal distribution with a gap.

This can suggest the data are grouped in some way and it may be difficult to summarise the data with single summary statistics. (Imagine Figure 3.2 represents heights of people on a school trip—what could explain the distribution looking gappy like that?)

In such cases, then it may be appropriate to give, for example, more than one measure of location.

3.2.2 Symmetry

The summary statistics we looked at previously were all measures of location or spread—they tell us nothing about the symmetry of the distribution.

There is another summary statistic called **skewness** which measures the *assymmetry* of a distribution.

The sample skewness for a sample $x_1, x_2, \ldots, x_n$, of observations is defined as:

$$g = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{x_i - \bar{x}}{s} \right)^3,$$

where $\bar{x}$ and s are the sample mean and standard deviation respectively.

A perfectly symmetric distribution has a skewness of zero.

A distribution with skewness greater than zero is said to be positively skewed, or skewed to the right (meaning the right 'tail' is longer).

A distribution with skewness less than zero is said to be negatively skewed, or skewed to the left (the left 'tail' is longer).

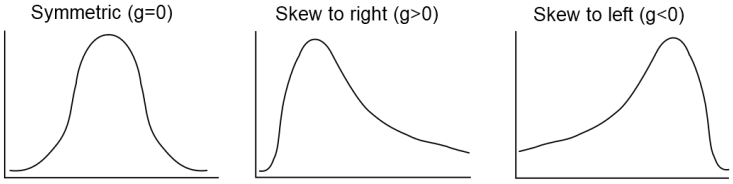


Figure 3.3: Symmetric and asymmetric (skewed) distributions.

3.2.3 Outliers

An outlier is an observation which is in some sense extreme. In the context of a single sample of observations on one random variable, outliers are observations that are well above or well below the other values in the data. For example, the observation of 3.83 in the Cavendish dataset considered in Section 2.3. All such extreme observations should be checked if possible to ensure they are correct values. It is important to identify any outliers in a data set as they can considerably distort numeric summaries or analytical methods (robustness).

In cases when an observation appears to be an outlier and no reason for the extreme measurement is found, the data could be analysed both with the outlier

included and once it has been removed. Thus the distortion due to the outlier can be fully assessed.

3.3 Basic plot types

3.3.1 Histogram and bar charts

Whenever more than about twenty observations are involved, it is often helpful to group the observations in a **frequency table**. Frequency tables are also helpful when constructing histograms as we shall see in a moment. We write f_i for the frequency of observation x_i $(i = 1, \ldots, k)$. A frequency table shows how many observations fall into various classes defined by categorising the observations into groups, see the Coursework marks example. The choice of which classes to use is somewhat arbitrary, but since it affects the visual impression given by the data when forming a histogram, the choice should be made with care.

The following are guidelines:

1. For continuous data, we usually choose consecutive intervals of the same width. For discrete data, the individual values are used if this is reasonable, but if the data are sparse it may be necessary to classify the observations into consecutive groups of values with the same number of values in each group. In either case, care is needed when specifying the intervals so that ambiguities are avoided.

2. Interval or group sizes should be chosen so that most frequencies (of observations in a class) are of a moderate size compared with the total number of observations. For example, data on the heights of 100 individuals which range from 160cm to 190cm might be grouped easily in intervals of 2cm or possibly 5cm but not 1mm or 50cm.

Once we have constructed a frequency table we can construct a **histogram** easily as the data have already been grouped. When drawing a histogram the classification intervals are represented by the scale on the abscissa ('x-axis') of a graph (N.B. sometimes the midpoints of the intervals are used as the scale on the abscissa) and rectangles are drawn on this base so that the *area* of the rectangle is *proportional to the frequency* of observations in the class. The unit on the ordinate ('y-axis') is the number of observations per unit class interval. Note that the *heights* of the rectangle will be *proportional to frequencies* if and only if class intervals of *equal* size are used.

Histograms are usually given in terms of *frequency* (number of occurrences) but can alternatively be given in terms of *density*. Density rescales the histogram so that the area in the rectangles sum to one. The shape of the histogram is thus not affected but the y-axis is rescaled. Frequency has a simple interpretation whereas density allows us to compare two samples of different size (heights of the population of Nottingham, approximately 337,000 individuals with heights

of the population of Long Eaton, approximately 39,000 individuals) and to compare with probability distributions.

Example 3.3.1. **IQ Scores** The I.Q. of 100 people chosen at random was measured, resulting in the following frequency table:

I.Q.	# of people (frequency)
$IQ \leq 80$	0
$80 < IQ \leq 90$	12
$90 < IQ \leq 100$	37
$100 < IQ \leq 110$	30
$110 < IQ \leq 120$	19
$120 < IQ \leq 130$	2

A histogram of these data is:

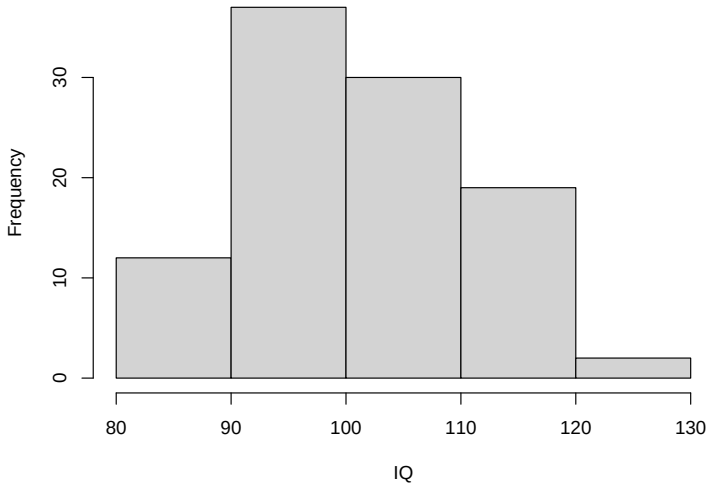


Figure 3.4: Histogram of the IQ data

Remember: frequency should be *proportional to area*, and so for unequal class widths one should plot the frequency density. For the IQ data, if we wanted 110-130 to be one class, compare:

When the data are discrete an alternative and better form of graphical representation is a **bar chart** with the heights of the bars representing frequencies, see Figure 3.6.

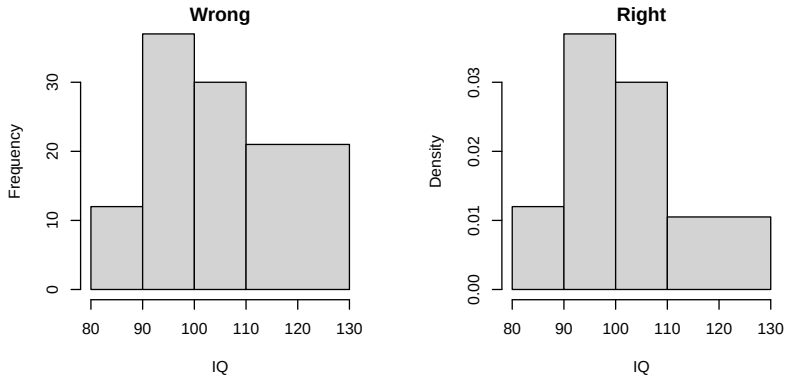


Figure 3.5: Histogram of IQ data with unequal bar widths: wrong and right versions

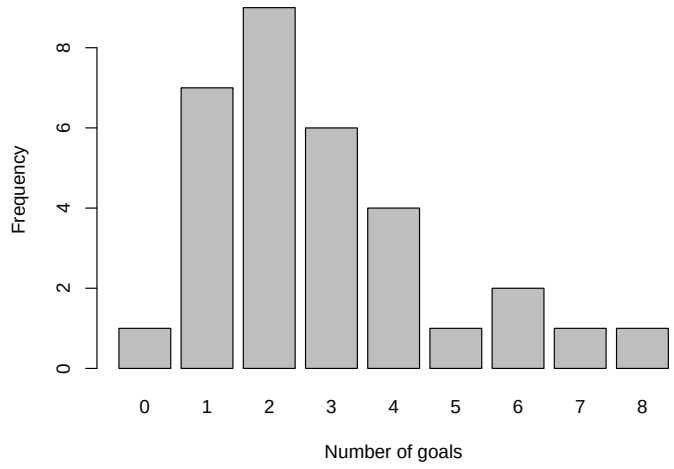


Figure 3.6: Goals scored in each of 32 FA Cup third round matches

3.3.2 Density plots

For continuous data, the histogram gives an approximation of the underlying distribution. The width and choice of endpoints of the intervals for the histogram affect the plot. Also for most continuous distributions we assume that a small change in value leads to a small change, up or down, in the likelihood of the value occurring. For example, the chance of an adult male being 169.9cm tall is unlikely to be very different to the chance of being 170.1cm tall. However, if we break the histogram into 5cm intervals with intervals 165cm-170cm and 170cm-175cm the height of the bars could be significantly different suggesting a big change in the likelihood of the heights.

In Figure 3.7 are 3 histograms for the same data, a sample of heights (cm) of 100 UK adult males. Histograms 1 and 3 use intervals of length $5cm$ but different starting points for the intervals. Histogram 2 uses intervals of length $2cm$.

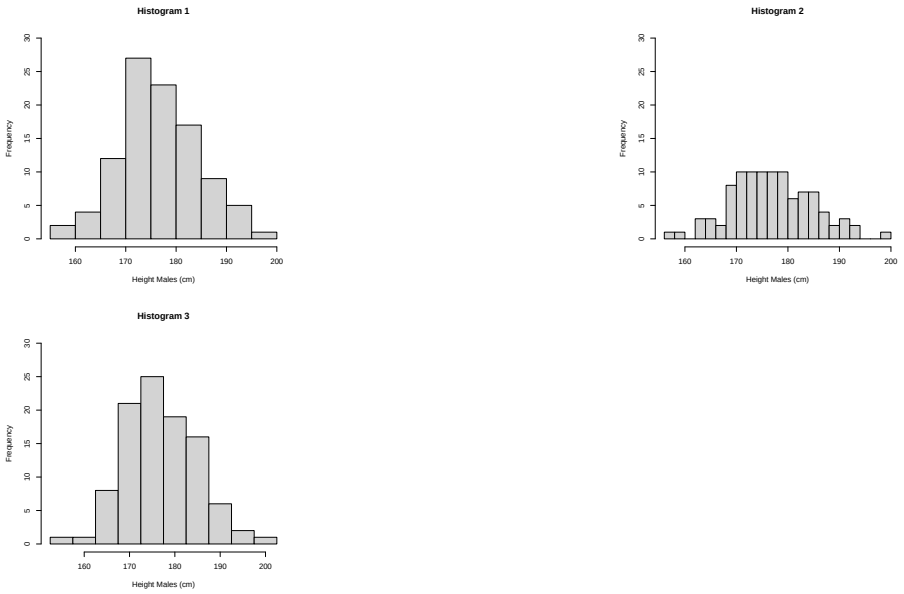


Figure 3.7: Histograms with different intervals

The heights (frequencies) differ between histograms 1 and 3 and histogram 2 due to the different interval widths. In Figure 3.8 we re-plot the histograms using density so the areas sum to 1 and we can perform a direct comparison.

An alternative to the histogram is a density plot. A density plot uses the data to estimate the distribution of the population using an approach known as *kernel smoothing*. Kernel smoothing estimates the probability density function (pdf) of the distribution of the population which is a measure of how likely a particular value is to occur. We will give a formal definition of the pdf in Section

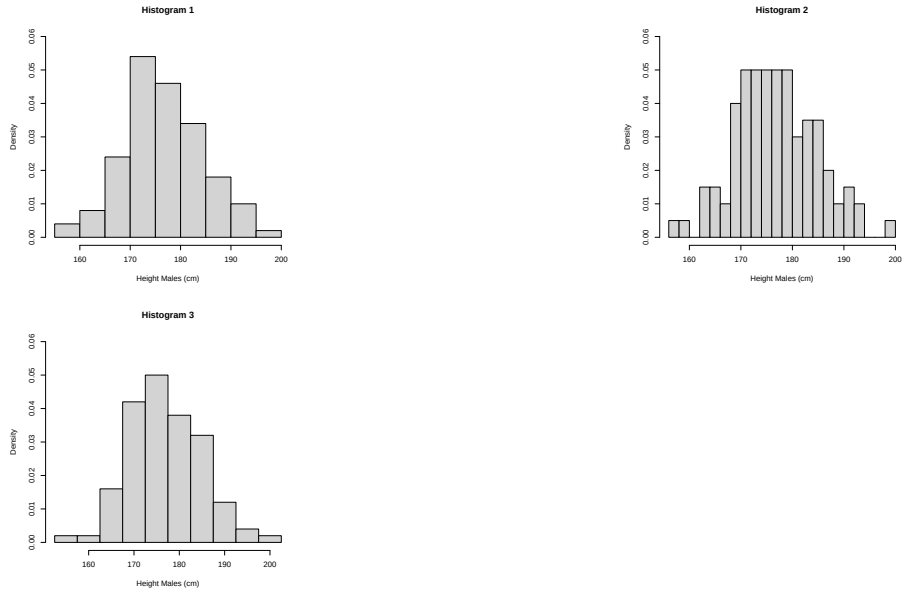


Figure 3.8: Histograms with different intervals

5.2. This approach removes the need to specify intervals for values as for the histogram and produces a continuous approximation of the density, how likely values are. In Figure 3.9, we illustrate with the UK adult male height data and also superimpose the density plot on histogram 1 to show the similarities.

NB. Histograms and density plots of data may not bear much resemblance to distribution of population when the sample size, n, is *small*, although as n increases the histogram and density plot should resemble the population distribution more closely.

In Figure 3.10, we plot histograms of random samples of sizes $n = 15, 100, 1000$ of UK adult males with the true population distribution's pdf superimposed (red).

The plots in Figure 3.10 are repeated in Figure 3.11 using density plot instead of histogram. We note that for small n the density plot (estimate of the pdf) is rather bumpy with multiple modes and we would probably prefer the stability and unimodality of the histogram, whereas for large n, the density plot (estimate of the pdf) offers a better approximation for the underlying continuous distribution (true population pdf).

The following **R** Shiny app allows you to investigate data features along with histograms and density plots further for a data set comprising of marks of 3 groups of students on a maths test.

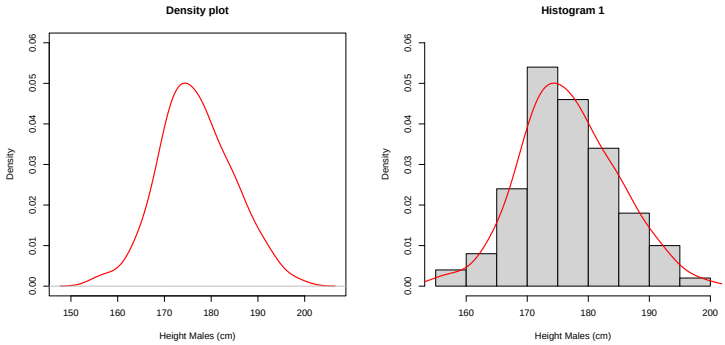


Figure 3.9: Histograms with different intervals

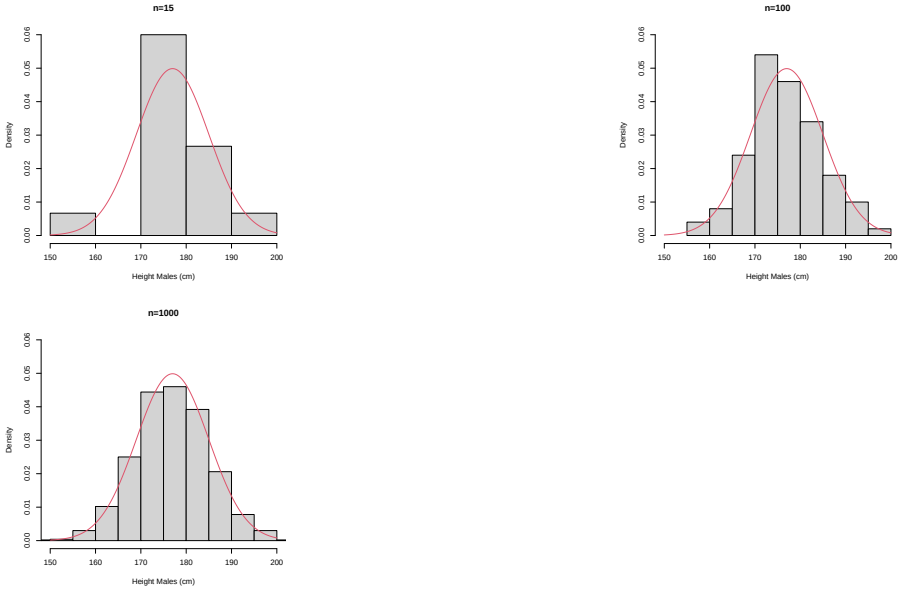


Figure 3.10: Histograms with different intervals

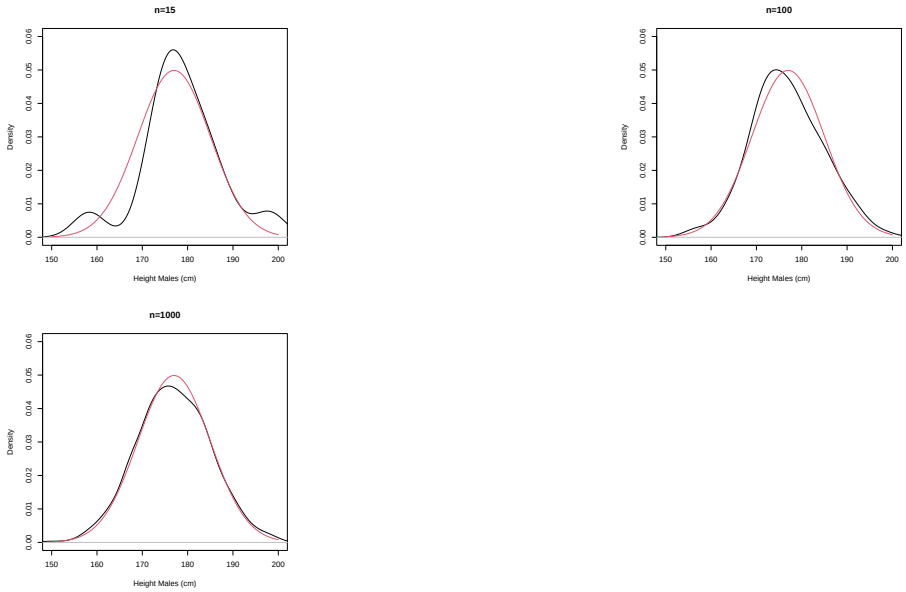


Figure 3.11: Density plots - sample (black) and population (red)

R Shiny app: Data Features

3.3.3 Boxplot

We have already seen that the lower quartile, median and upper quartile split the data into four portions. Together with the lowest value in the sample and the highest value in the sample, these statistics form the *five-number summary*:

Example 3.3.2. **Coursework marks**
The *five-number summary* for the coursework marks data given in Section 1.4 are:

min	Q_1	median	Q_3	max
34	44	46	48	50

Between each statistic fall 25% of the observations. The simplest form of the **boxplot** is simply a visual presentation of the five number summary as follows:

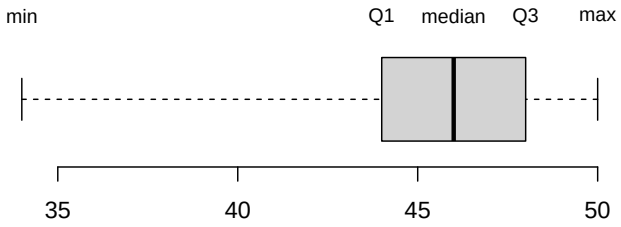


Figure 3.12: A boxplot depicting the five-number summary

Here the box is drawn with its left hand edge at the lower quartile and right hand edge at the upper quartile. A line is drawn at the median that divides the box in two. From the centre of each end of the box, a line is drawn to the minimum and maximum of the values in the sample. These lines are sometimes called **whiskers** and the plots are sometimes called box-and-whisker plots. There are other variations of the boxplot but this is the simplest version. Sometimes extreme observations called **outliers** (see later) are picked out and denoted with either a '*' or 'o' to stop them from influencing the whiskers too much. In fact, the `boxplot` function in **R** does this by default:

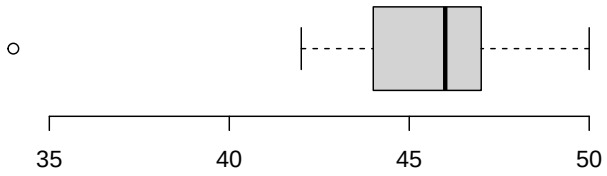


Figure 3.13: A boxplot with an outlier picked out

3.3.4 Cumulative frequency diagrams, and the empirical CDF

The **cumulative frequency** at x is defined as the number of observations less than or equal to x. The *relative* cumulative frequency, often written as $\hat{F}(x)$, is the cumulative frequency of x divided by the total number of observations n.

$\hat{F}(x)$ is also called the **empirical cumulative distribution function** (empirical cdf). The cumulative distribution function (cdf) for the population, denoted $F(x)$, is the probability of observing an observation in the population taking a value less than or equal to x. $F(x)$ is an increasing (strictly non-decreasing) function in x with the rate of change in the cdf determined by the pdf introduced in discussions of the density plot. We will introduce the cdf formally in Section 5.2.

A cumulative frequency diagram involves plotting the cumulative frequency at x versus x. If the data are grouped continuous data (IQ scores) then straight lines are drawn between the upper class boundaries, and if the data are discrete,goals per FA cup match, Figure 3.6, or ungrouped data then a step function is used. This is illustrated in Figure 3.14.

Example 3.3.3. **IQ Scores (revisited)**
The cumulative frequency and relative cumulative frequency for the I.Q. data above are:

x	Cum. freq.	$\hat{F}(x)$
80	0	0
90	12	0.12
100	49	0.49
110	79	0.79
120	98	0.98
130	100	1.00

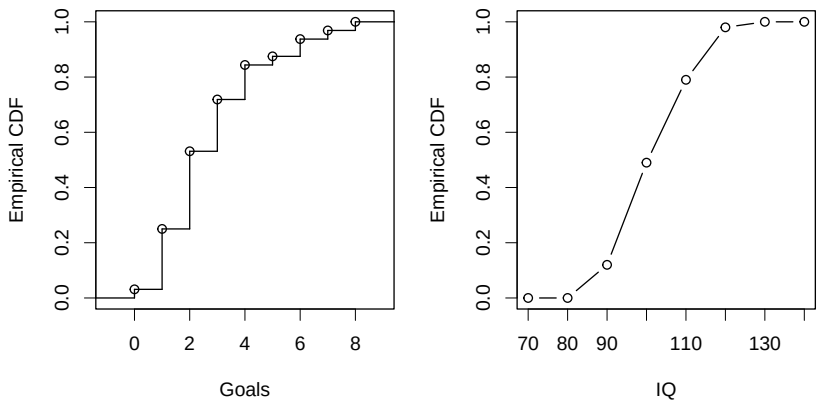


Figure 3.14: Empirical cdf plots for the 'Goals' and 'IQ' data sets

The median can be estimated from a cumulative frequency diagram by finding the value x corresponding to cumulative frequency of $n/2$ (or $\hat{F}(x) = 0.5$ if using the empirical CDF).

In Video 5 we study comparing the empriical distribution (pdf and cdf) with the random variable (population) the observations come from. This comparison is done using an **R Shiny** app which gives the histogram and estimate of the probability density function. A link to the **R Shiny** app is provided after the video to allow you to explore these features for yourself.

Watch Video 5: Empirical pdf and cdf

R Shiny app: pdf-cdf-QQ

3.3.5 Stem and leaf

One way of representing both discrete or continuous data is to use a **stem-and-leaf plot**. This plot is similar to a bar chart/histogram but contains more

information. It is best described by way of an example.

Example 3.3.4. **Seeds data**
In the routine testing of consignments of seeds, the following procedure is used. From a consignment 100 seeds are selected and kept under controlled conditions. The number of seeds which have germinated after 14 days is counted. This procedure is repeated 40 times with the following results:

88	87	85	91	93	91	94	87	90	91
92	87	91	89	87	90	88	85	90	92
89	86	91	92	91	91	93	93	87	90
91	91	89	90	90	91	91	93	92	85

The range of data is $94 - 85 = 9$ and we divide this range into intervals of fixed length as we would for a histogram.

For a stem-and-leaf plot we usually make the class interval either 0.5, 1 or 2 times a power of ten and aim for between 4 and 10 intervals. Of course, this is sometimes not possible for very small data sets. For these data an interval of two seems appropriate as this will give us 5 or 6 intervals. Next we draw a vertical line. On the left of this vertical line we mark the interval boundaries in increasing order but note only the first few digits that are in common to the observation in the interval. This is called the **stem**. We then go through the observations one by one, noting down the next significant digit on the right-hand side of the appropriate stem. This forms the **leaves**. Here we obtain:

8	|	5	5	5													
8	|	7	7	7	7	6	7										
8	|	8	9	8	9	9											
9	|	1	1	0	1	1	0	0	1	1	1	0	1	1	0	0	1	1
9	|	3	2	2	2	3	3	3	2									
9	|	4																

The first stem (line) contains any values of 84 and 85, the second stem of 86 and 87, and so on. Note that by allowing the first stem to represent 84 & 85 we have ensured that there are stems for 88 & 89 and 90 & 91 and no stem for 89 & 90 — a stem which would be very difficult to enter on a plot! A final version of the plot is found by ordering the digits within each stem. For these data the final stem-and-leaf plot is

8	|	5	5	5													
8	|	6	7	7	7	7	7										
8	|	8	8	9	9	9											
9	|	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1
9	|	2	2	2	2	3	3	3	3								
9	|	4															

3.3.6 Pie charts

When we wish to display proportions of observations in a sample that take each of a discrete number of values, a **pie chart** is sometimes used:

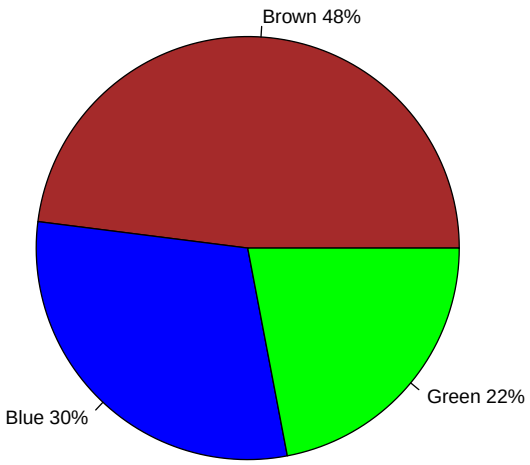


Figure 3.15: Pie chart of eye colour of people in Britain

However, there are many drawbacks with pie charts, especially when the number of categories is large, or when some categories have small frequencies, and the comparison of groups with similar proportions is difficult. If you're thinking about using a pie chart then I suggest: stop, and ask yourself whether a bar chart would be clearer!

Figure 3.16 is a pie chart showing the proportion of oil production by different OPEC countries in 2016.

And Figure 3.17 is a bar chart showing the same data. Which do you find the clearer?

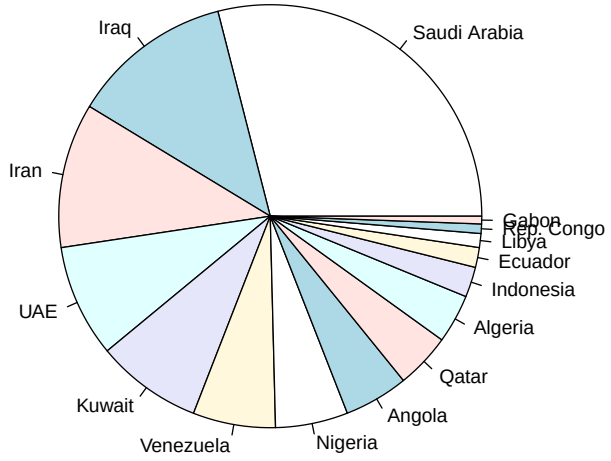


Figure 3.16: Pie chart of oil production by OPEC members

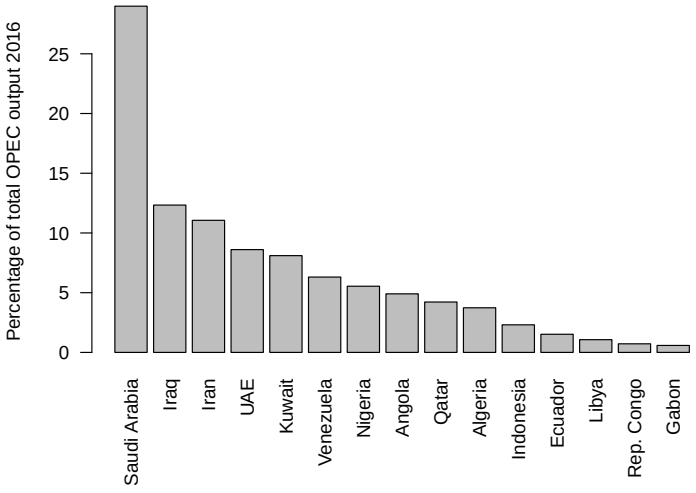


Figure 3.17: Bar chart of oil production by OPEC members

3.3.7 Dotplots

A **dotplot** displays each data value as a dot, and is used for both continuous and discrete data. It is usually used only when the sample size is small, otherwise the plot quickly gets overcrowded. Here is a dotplot for the $n = 29$ Cavendish data values.

Figure 3.18: Simple dot plot of the Cavendish data

The 'overplotting' makes it difficult to see how many data values there are in the middle of the data set. Sometimes to make things a bit clear some 'jitter' (randomness) is added in the y direction and/or the points are made slightly transparent, both of which help a lot in this case:

Figure 3.19: Dot plot of the Cavendish data with some jitter and transparency

For discrete data the dots are stacked above the horizontal axis. The result is something similar to a bar chart, but showing individual points. Here is a dotplot for the seed data:

3.3.8 Scatterplots

In addition to displaying the data on each random variable as above, when we have data that consists of observations on two or more random variables, it is useful to try and assess any relationships between random variables by using a **scatterplot**. A scatterplot is simply a graph with one random variable as abscissa and another random variable as ordinate. A point is plot on the graph for each element of data at the observed values of the two random variables,see Figure 3.21.

This is very useful for exploring the relationship between two variables. In the above example we observe that the number of seeds which germinate increases linearly with temperature. We can extend the approach to comparing more than

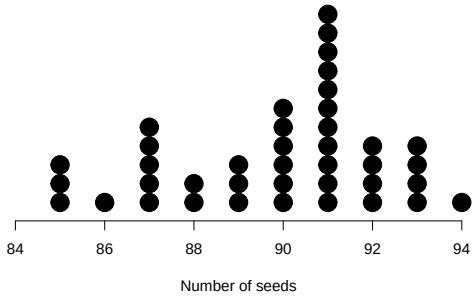


Figure 3.20: Dot plot of some discrete seed count data

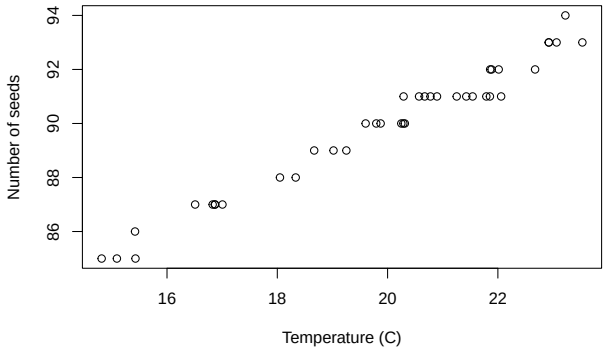


Figure 3.21: Scatter plot of number of seeds versus average temperature (40 observations)

two variables by producing a **scatterplot matrix** which consists of scatterplots for every pair of random variables, see Figure 3.22.

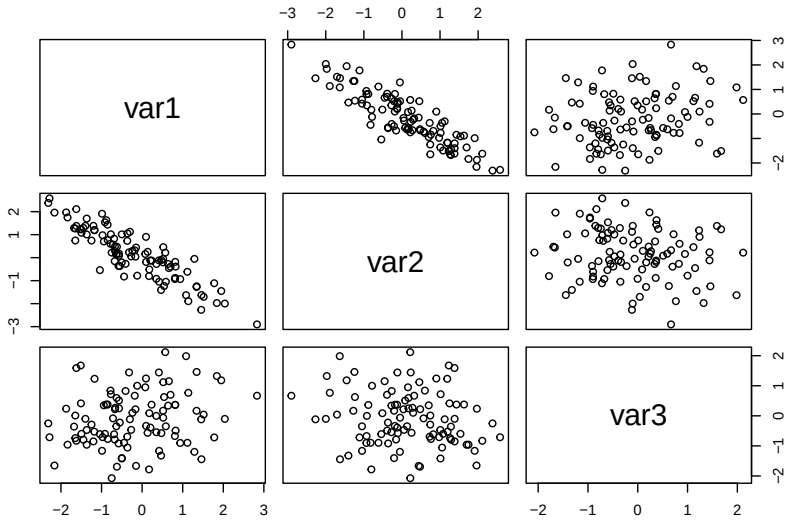


Figure 3.22: A scatterplot matrix for three variables (100 observations)

3.3.9 Summary

Histogram/Dotplot

Pros: Gives a good impression of the distribution of the data.

Cons: The histogram is sensitive to the classes chosen to group observations – giving only a vague impression of the data.

Density plot

Pros: Represents continuous distribution by a continuous function (density) aoviding the discretisation of histograms.

Cons: Over-interprets individual observations for small sample sizes often leading to erroneous multi-modality.

Boxplot

Pros: Good for comparing different samples or groups of observations on the same random variable. Gives a good quick summary of the data.

Cons: Gives no feel for the number of observations involved. Hides multiple modes.

Stem and leaf plot

Pros: Gives indication of general shape and other distributional features while allowing actual data values to be recovered.

Cons: Difficult to use for comparative purposes – suffers from lack of clarity.

Pie chart

Pros: Looks nice.

Cons: Only useful for comparing the relative proportions of observations in a small number of categories. Difficult to compare categories with similar frequencies, or very small frequencies.

3.4 Commenting on data

When we describe a data set in words, often to complement a plot, here are some things worth commenting about:

- *Location* - what is a typical value?
- *Spread* - how dispersed are the observations?
- *Multiple modes* - is there one or more 'peaks' (and why)?
- *Symmetry/skewness* - is skewness positive, negative, roughly zero?
- *Outliers* - are there any unusual observations?
- *Any other interesting patterns or features* - e.g. are two variables related?

We have given an overview of summarising data, both numerically (location and spread) and graphically. We are now in position to consider the mathematical underpinnings of statistics through the introduction of probability.

Task: Session 2

In Section 24, an introduction using to **R Markdown** is given.

Work through Section 24 and then attempt to complete the **R Markdown** file for Session 2:
Session 2: Plots in R

Chapter 4

Probability

4.1 Overview

In this Chapter we introduce **probability** as a **measure** associated with a **random experiment**. After providing a short motivation for probability (Section 4.2), we begin in Section 4.3 with the notion of a **Sample space** (Section 4.3), the set of possible outcomes of a random experiment and **Events** (Section 4.4), the outcome(s) which occur. This enables us in Section 4.5 to define **probability** as a finite measure which uses the scale 0 (impossible) to 1 (certain) to define the likelihood of an event. We conclude the chapter by introducing the concept of **conditional probability** (Section 4.6), the probability of one event **given** (conditional upon) another event (or events) having occurred. We present the key results of the Theorem of total probability and Bayes' formula. The discussion of conditional probability leads us naturally to consider the dependence between two (or more) events and the notion of **independence**, where the probability of an event occurring is not affected by whether or not another event has occurred and we explore this further in Section 4.7.

4.2 Motivation

There are many situations where we have uncertainty and want to quantify that uncertainty.

(a) Manchester United will win the Premier League this season.

(b) The Labour Party will win the next general election.

(c) The £ will rise against the $ today.

(d) Coin tossed repeatedly - a head will turn up eventually.

(e) In 5 throws of a dart, I will hit the Bull's eye once.

(f) If I play the lottery every week I will win a prize next year.

(a)-(c) are subjective probabilities, whereas (d)-(f) are objective/statistical/physical probabilities.

The general idea is:

(a) A conceptual random experiment $\mathcal{E}$.

(b) List all possible outcomes Ω for the experiment $\mathcal{E}$ but **don't know** which occurs, has occurred or will occur.

(c) Assign to each possible outcome ω a real number which is the probability of that outcome.

4.3 Sample Space

We begin by defining a *set*.

Definition 4.3.1. **Set.**
A *set* is a collection of objects. The notation for a set is to simply list every object separated by commas, and to surround this list by curly braces { and }. The objects in a set are referred to as the *elements* of the set.

There is no restrictions on what constitutes as an object in set. A set can have a finite or infinite number of elements. The ordering of the elements in a list is irrelevant. Two sets are equal if and only if they have the same collection of elements.

Definition 4.3.2. **Sample space.**
The *sample space* Ω for a random experiment $\mathcal{E}$ is the set of all possible outcomes of the random experiment.

Example 4.3.3. **Rolling a die.**

The sample space for the roll of a die is

$$\Omega = \{1, 2, 3, 4, 5, 6\},$$

that is, the set of the six possible outcomes.

Example 4.3.4. **Dart in a target.**

Dart into a circular target, radius 1:

$$\Omega = \{(x, y) : x^2 + y^2 \leq 1\},$$

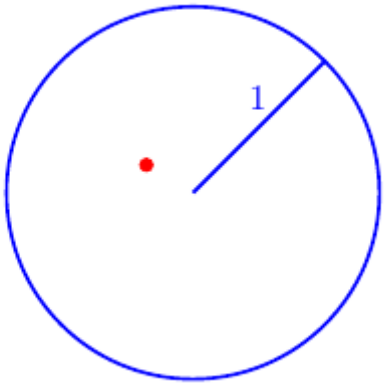


Figure 4.1: Example: $(x, y) = (-0.25, 0.15)$.

that is, the set of pairs of real numbers that are less than a distance 1 from the origin $(0, 0)$.

Note that the examples illustrate how Ω may be discrete or continuous.

4.4 Events

Definition 4.4.1. **Event.**
An *event* relating to an experiment is a subset of Ω.

Example 4.4.2. **Toss two coins.**

The sample space for the toss of two fair coins is

$$\Omega = \{HH, HT, TH, TT\}.$$

Let A be the event that at least one head occurs, then

$$A = \{HH, HT, TH\}.$$

Note that the events HT (Head on coin 1 and Tail on coin 2) and TH (Tail on coin 1 and Head on coin 2) are distinct events.

Example 4.4.3. **Volcano eruption.**

The sample space of time in years until a volcano next erupts is

$$\Omega = \{t : t > 0\} = (0, \infty),$$

that is, all positive real numbers. Let event L be the volcano erupting in the next 10 years, then

$$L = \{t : 0 < t \leq 10\} = (0, 10].$$

We summarise key set notation, involving sets E and F, below:

1. We use $\omega \in E$ to denote that ω is an element of the set E. Likewise, $\omega \notin E$ denotes that ω is not an element of E;

2. The notation $E \subseteq F$ means that if $\omega \in E$, then $\omega \in F$. In this case, we say E is a *subset* of F;

3. E^c - complement of E, sometimes written $\bar{E}$.
   E^c consists of all points in Ω that are not in E. Thus, E^c occurs if and only if E does not occur, see Figure 4.2.

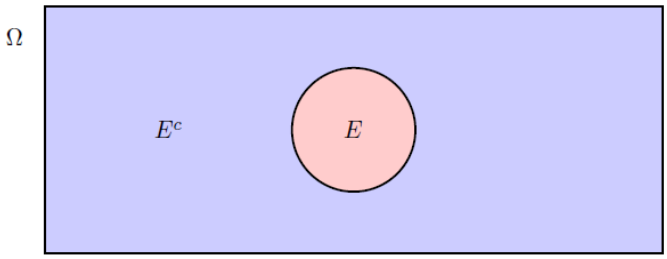


Figure 4.2: Complement example.

4. The *intersection* of two sets E and F, denoted $E \cap F$, is the set of all elements that belong to both E and F, see Figure 4.3.

5. If $E \cap F = \emptyset$ then E and F cannot both occur, *i.e.* E and F are *disjoint* (or *exclusive*) sets, see Figure 4.4.

6. The *union* of two sets E and F, denoted $E \cup F$, is the set of all elements that belong to either E or to F, see Figure 4.5.

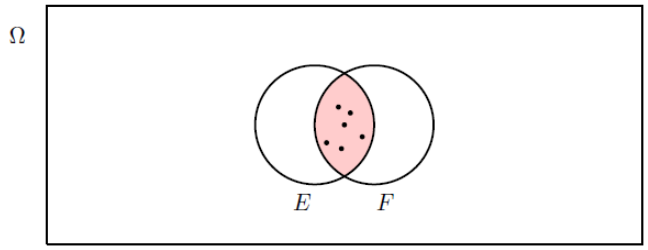


Figure 4.3: Intersection example.

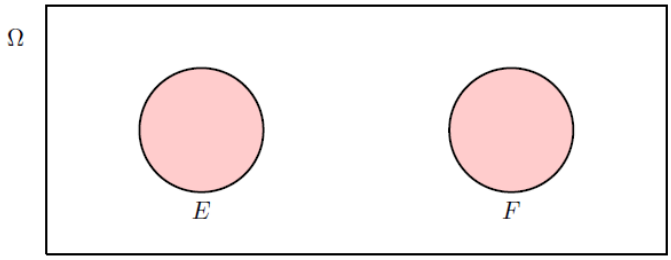


Figure 4.4: Disjoint (exclusive) example.

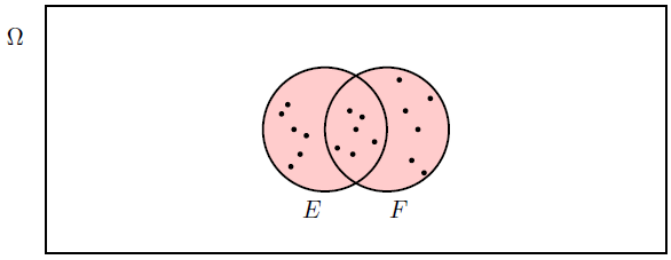


Figure 4.5: Union example.

7. The set $\{\}$ with no elements in it is called the *empty set* and is denoted $\emptyset$. **Note**: $\Omega^c = \emptyset$ and $\emptyset^c = \Omega$.

A summary of sets notation using the outcomes from a six sided die are presented in the Video 6.

Watch Video 6: Set notation

4.5 Probability

There are different possible interpretations of the meaning of a probability:

- **Classical interpretation.** Assuming that all outcomes of an experiment are equally likely, then the probability of an event $A = \frac{n(A)}{n(\Omega)}$, where $n(A)$ is the number of outcomes satisfying A and $n(\Omega)$ is the number of outcomes in Ω (total number of possible outcomes).
- **Frequency interpretation.** The probability of an event is the relative frequency of observing a particular outcome when an experiment is repeated a large number of times under similar circumstances.
- **Subjective interpretation.** The probability of an event is an individual's perception as to the likelihood of an event's occurrence.

Definition 4.5.1. **Probability.**

A *probability* (*measure*) is a real-valued set function P defined on the events (subsets) of a sample space Ω satisfying the following three axioms (see Kolmogorov, 1933):

1. $P(E) \geq 0$ for any event E;
2. $P(\Omega) = 1$;
3. If $E_1, E_2, \ldots, E_n$ are disjoint events (i.e. $E_i \cap E_j = \emptyset$ for all $i \neq j$), then

$$P\left(\bigcup_{i=1}^{n} E_i\right) = \sum_{i=1}^{n} P(E_i).$$

If Ω is *infinite* then 3. can be extended to:
3'. If $E_1, E_2, \ldots$ is any infinite sequence of disjoint events (i.e. $E_i \cap E_j = \emptyset$ for all $i \neq j$), then

$$P\left(\bigcup_{i=1}^{\infty} E_i\right) = \sum_{i=1}^{\infty} P(E_i).$$

Note that all of the other standard properties of probability (measures) that we use are derived from these three axioms.

Example 4.5.2.
Using only the axioms above, prove:

- $0 \leq P(E) \leq 1$ for any event E;
- $P(E^C) = 1 - P(E)$ where E^C is the complement of E;
- $P(\emptyset) = 0$;
- $P(A \cup B) = P(A) + P(B) - P(A \cap B)$.

A summary of probability along with proofs of the results in Example 4.5.2 are provided in Video 7.

Watch Video 7: Probability

Solution to Example 4.5.2.

Since for any event E, $\Omega = E \cup E^c$, we have by axiom 2 that

$$1 = P(\Omega) = P(E \cup E^c).$$

By axiom 3, since E and E^c are disjoint events, we have that

$$1 = P(E \cup E^c) = P(E) + P(E^c).$$

which rearranges to give $P(E^c) = 1 - P(E)$.

Special cases
If $E = \emptyset$, then $E^c = \Omega$ giving $1 = P(\emptyset) + 1$ and it follows that $P(\emptyset) = 0$.
Since $P(E^c) \geq 0$, we have that $P(E) \leq 1$ and hence $0 \leq P(E) \leq 1$.

To study $P(A \cup B)$, we note that $A \cup B$ is formed by the union of the disjoint events: $A \cap B^c$, $A \cap B$ and $A^c \cap B$. Therefore using axiom 3,

$$P(A \cup B) = P(A \cap B^c) + P(A \cap B) + P(A^c \cap B).$$

Similarly, we have that

$$P(A) = P(A \cap B^c) + P(A \cap B)$$

and

$$P(B) = P(A \cap B) + P(A^c \cap B).$$

Since $P(A^c \cap B) = P(B) - P(A \cap B)$, we have that

$$\begin{aligned} P(A \cup B) &= P(A \cap B^c) + P(A \cap B) + P(A^c \cap B) \\ &= P(A) + P(B) - P(A \cap B) \\ &= P(A) + P(B) - P(A \cap B). \end{aligned}$$

In many cases, Ω consists of $N(= n(\Omega))$ equally likely elements, *i.e.*

$$\Omega = \{\omega_1, \omega_2, \ldots, \omega_N\},$$

with $P(\omega_i) = \frac{1}{N}$.

Then, for any event E (*i.e.* subset of Ω),

$$P(E) = \frac{n(E)}{n(\Omega)} = \frac{n(E)}{N}$$

coinciding with the Classical interpretation of probability.

Example 4.5.3.
1. **Throw a die.** $\Omega = \{1, 2, 3, 4, 5, 6\}$.

$$P(\{1\}) = P(\{2\}) = \ldots = P(\{6\}) = \frac{1}{6}.$$

The probability of throwing an odd number is

$$P(\text{Odd}) = P(\{1, 3, 5\}) = \frac{3}{6} = \frac{1}{2}.$$

2. **Draw a card at random from a standard pack of 52.**

$$\Omega = \{A\clubsuit, 2\clubsuit, 3\clubsuit, \ldots, K\diamondsuit\}.$$

$P(\omega) = 1/52$ for all $\omega \in \Omega$.
If $E = \{\text{Black}\}$ and $F = \{\text{King}\}$, then there are 26 black cards, $n(E) = 26$, 4 kings, $n(F) = 4$ and 2 black kings ($K\clubsuit$ and $K\spadesuit$), $n(E \cap F) = 2$,

$$\begin{aligned} P(E \cup F) &= P(E) + P(F) - P(E \cap F) \\ &= \frac{26}{52} + \frac{4}{52} - \frac{2}{52} \\ &= \frac{7}{13}. \end{aligned}$$

4.6 Conditional probability

Definition 4.6.1. **Conditional Probability.**

The *conditional probability* of an event E *given* an event F is

$$P(E \mid F) = \frac{P(E \cap F)}{P(F)}, \quad \text{provided } P(F) > 0.$$

Note if $P(F) > 0$, then $P(E \cap F) = P(E|F)P(F)$.

Moreover, since $E \cap F = F \cap E$, we have that

$$P(E|F)P(F) = P(E \cap F) = P(F \cap E) = P(F|E)P(E).$$

In other words, to compute the probability of both events E and F occurring, we can either:

- Consider first whether E occurs, $P(E)$, and then whether F occurs *given* that E has occurred, $P(F|E)$,
- Or consider first whether F occurs, $P(F)$, and then whether E occurs *given* that F has occurred, $P(E|F)$.

Example 4.6.2. **Rolling a die.**

Consider the experiment of tossing a fair 6-sided die. What is the probability of observing a 2 if the outcome was even?

Let event T be observing a 2 and let event E be the outcome is even. Find $P(T|E)$:

$$P(T|E) = \frac{P(T \cap E)}{P(E)} = \frac{1/6}{1/2} = \frac{1}{3}.$$

Definition 4.6.3. **Independence.**

Two events E and F are independent if

$$P(E \cap F) = P(E)P(F).$$

Theorem 4.6.4.
If $P(F) > 0$, two events, E and F, are independent if and only if $P(E|F) = P(E)$.

$$\begin{aligned} & P(E|F) = P(E) \\ \iff \quad & \frac{P(E \cap F)}{P(F)} = P(E) \\ \iff \quad & P(E \cap F) = P(E)P(F) \\ \iff \quad & E \text{ and } F \text{ are independent.} \end{aligned}$$

Observations on Independence

- If E and F are **NOT** independent then

$$P(E \cap F) \neq P(E)P(F).$$

- E and F being independent is **NOT** the same as E and F being disjoint.

Independence: $P(E \cap F) = P(E)P(F)$.
Disjoint (exclusive): $P(E \cap F) = P(\emptyset) = 0$.

Example 4.6.5. **Rolling a die.**

Consider the experiment of tossing a fair 6-sided die.
Let $E = \{2, 4, 6\}$, an even number is rolled on the die and $F = \{3, 6\}$, a multiple of 3 is rolled on the die.

Are E and F independent?

$E \cap F = \{6\}$, so $P(E \cap F) = \frac{1}{6}$.

$$P(E) \times P(F) = \frac{3}{6} \times \frac{2}{6} = \frac{1}{6} = P(E \cap F)$$

Therefore E and F are independent.

Definition 4.6.6. **Partition.**

A *partition* of a sample space Ω is a collection of events $E_1, E_2, \ldots, E_n$ in Ω such that:

i. $E_i \cap E_j = \emptyset$ for all $i \neq j$ (disjoint sets)

ii. $E_1 \cup E_2 \cup \ldots \cup E_n = \bigcup_{i=1}^{n} E_i = \Omega$.

We can set $n = \infty$ in Definition 4.6.6 and have infinitely many events constructed the partition.

Figure 4.6 presents an example of a partition of Ω using six events $E_1, E_2, \ldots, E_6$.

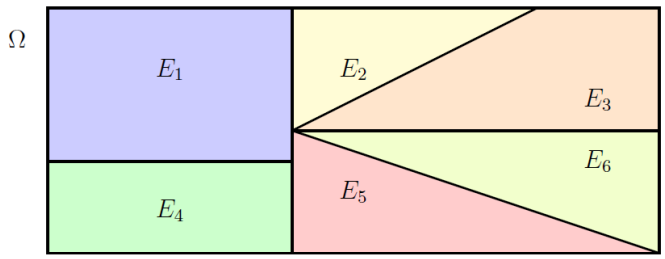


Figure 4.6: Example of a partition of a sample space using six events.

For an event $F \subseteq \Omega$,

$$F = (F \cap E_1) \cup (F \cap E_2) \cup \ldots \cup (F \cap E_n).$$

This is illustrated in Figure 4.7 using the partition given in Figure 4.6.

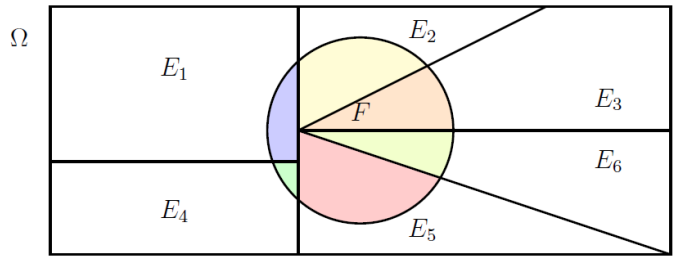


Figure 4.7: The event *F* expressed in terms of the union of events.

Theorem 4.6.7. **Theorem of Total Probability.**

Let $E_1, E_2, \ldots, E_n$ be a partition of Ω (i.e. $E_i \cap E_j = \emptyset$ for all $i \neq j$ and $\bigcup_{i=1}^{n} E_i = \Omega$) and let $F \subseteq \Omega$ be any event. Then,

$$P(F) = \sum_{i=1}^{n} P(F \mid E_i)\, P(E_i).$$

Since the E_i's form a partition:

1. $F = F \cap \Omega = \bigcup_{i=1}^{n} [F \cap E_i]$.
2. For each $i \neq j$, $[F \cap E_i] \cap [F \cap E_j] = \emptyset$.

Therefore

$$P(F) = \sum_{i=1}^{n} P\left(F \cap E_i\right). \tag{4.1}$$

By the definition of conditional probability, for each i,

$$P\left(F \cap E_i\right) = P(F|E_i)P(E_i). \tag{4.2}$$

Substituting (4.2) into (4.1) completes the proof.

Example 4.6.8. **Tin can factory.**

Suppose that a factory uses three different machines to produce tin cans. Machine I produces 50% of all cans, machine II produces 30% of all cans and machine III produces the rest of the cans. It is known that 4% of cans produced on machine I are defective, 2% of the cans produced on machine II are defective and 5% of the cans produced on machine III are defective. If a can is selected at random, what is the probability that it is defective?

Let event M_i be the can is produced by machine i, $i = 1, 2, 3$. Let D be the event that the can is defective. From the question, we know

$$\begin{array}{rclrcl} P(M_1) & = & 0.5, & P(D|M_1) & = & 0.04, \\ P(M_2) & = & 0.3, & P(D|M_2) & = & 0.02, \\ P(M_3) & = & 0.2, & P(D|M_3) & = & 0.05. \end{array}$$

Therefore

$$\begin{array}{rcl} P(D) & = & \displaystyle\sum_{i=1}^{3} P(D|M_i)P(M_i) \\ & = & (0.04 \times 0.5) + (0.02 \times 0.3) + (0.05 \times 0.2) \\ & = & 0.036. \end{array}$$

Example 4.6.9. **Job interview problem.**

A manager interviews 4 candidates for a job. The manager **MUST** make a decision offer/reject after each interview. Suppose that candidates are ranked $1, 2, 3, 4$ (1 best) and are interviewed in random order.

The manager interviews and rejects the first candidate. They then offer the job to the first candidate that is better than the rejected candidate. If all are worse then they offer the job to the last candidate.

What is the probability that the job is offered to the best candidate?

Attempt Example 4.6.9 (Job interview problem) and then watch Video 8 for the solution.

Watch Video 8: Job Interview

Solution to Example 4.6.9 (Job interview problem).

Let F be the event that the best candidate is offered the job.

For $k = 1, 2, 3, 4$, let E_k be the event that candidate k (the k^{th} best candidate) is interviewed first. Note that E_ks form a partition of the sample space and by randomness,

$$P(E_1) = P(E_2) = P(E_3) = P(E_4) = \frac{1}{4}.$$

We have that:
1. $P(F|E_1) = 0$. If the 1^{st} ranked candidate is interviewed first they will be rejected and cannot be offered the job.
2. $P(F|E_2) = 1$. If the 2^{nd} ranked candidate is interviewed first then all candidates will be rejected until the best (1^{st} ranked) candidate is interviewed and offered the job.
3. $P(F|E_3) = \frac{1}{2}$. If the 3^{rd} ranked candidate is interviewed first then whoever is interviewed first out of the 1^{st} ranked and 2^{nd} ranked candidates will be offered the job. Each of these possibilities is equally likely.
4. $P(F|E_4) = \frac{1}{3}$. If the 4^{th} ranked (worst) candidate is interviewed first then the 1^{st} ranked candidate will only be offered the job if they are interviewed second.

By the Theorem of Total Probability,

$$\begin{aligned} P(F) &= \sum_{i=1}^{4} P(F|E_i)P(E_i) \\ &= P(F|E_1)P(E_1) + P(F|E_2)P(E_2) + P(F|E_3)P(E_3) + P(F|E_4)P(E_4) \\ &= 0 \times \frac{1}{4} + 1 \times \frac{1}{4} + \frac{1}{2} \times \frac{1}{4} + \frac{1}{3} \times \frac{1}{4} \\ &= \frac{11}{24}. \end{aligned}$$

Theorem 4.6.10. **Bayes Formula.**

Let $E_1, E_2, \ldots, E_n$ be a partition of Ω, *i.e.* $E_i \cap E_j = \emptyset$ for all $i \neq j$ and $\bigcup_{i=1}^{n} E_i = \Omega$, such that $P(E_i) > 0$ for all $i = 1, \ldots, n$, and let $F \subseteq \Omega$ be any event such that $P(F) > 0$. Then

$$P(E_k|F) = \frac{P(F|E_k)P(E_k)}{\sum_{i=1}^{n} P(F|E_i)P(E_i)}.$$

If $P(F) > 0$ and $P(E_k) > 0$, then by definition

$$P(E_k|F) = \frac{P(E_k \cap F)}{P(F)} = \frac{P(F|E_k)P(E_k)}{P(F)}.$$

Since $E_1, E_2, \ldots, E_n$ is a partition of Ω such that $P(E_i) > 0$ for all i, then by the Theorem of Total Probability we can rewrite $P(F)$ and obtain

$$P(E_k|F) = \frac{P(F|E_k)P(E_k)}{\sum_{i=1}^{n} P(F|E_i)P(E_i)}.$$

Example 6.11. **Tin can factory (continued).**

Consider Example 4.6.8. Suppose now that we randomly select a can and find that it is defective.

What is the probability that it was produced by machine I?

$$P(M_1|D) = \frac{P(D|M_1)P(M_1)}{P(D)} = \frac{0.04 \times 0.5}{0.036} = 0.55.$$

Example 4.6.12. **Guilty?**

At a certain stage of a jury trial a jury member gauges that the probability that the defendant is guilty is 7/10.

The prosecution then produces evidence that fibres of the victim's clothing were found on the defendant.

If the probability of such fibres being found is 1 if the defendant is guilty and 1/4 if the defendant is not guilty, what now should be the jury member's probability that the defendant is guilty?

Attempt Example 4.6.12 (Guilty?) and then watch Video 9 for the solution.

Watch Video 9: Guilty?

Solution to Example 4.6.12 (Guilty?)

Let G be the event that the defendant is guilty and let F be the event that fibres are found on the victim's clothing.

We want $P(G|F)$, the probability of being guilty **given** fibres are found on the victim's clothing.

We have that $P(G) = 0.7$, $P(G^c) = 1 - P(G) = 0.3$, $P(F|G) = 1$ and $P(F|G^c) = 0.25$.

Therefore, by Bayes' Theorem,

$$\begin{aligned} P(G|F) &= \frac{P(F \cap G)}{P(F)} \\ &= \frac{P(F|G)P(G)}{P(F|G)P(G) + P(F|G^c)P(G^c)} \\ &= \frac{1 \times 0.7}{1 \times 0.7 + 0.25 \times 0.3} \\ &= 0.9032. \end{aligned}$$

4.7 Mutual Independence

We can extend the concept of independence from two events to N events.

Definition 4.7.1. **Mutual independence.**

Events $E_1, E_2, \ldots, E_N$ are (mutually) *independent* if for *any* finite subset $\{i_1, i_2, \ldots, i_n\} \subseteq \{1, \ldots, N\}$,

$$P\left(\bigcap_{j=1}^{n} E_{i_j}\right) = \prod_{j=1}^{n} P(E_{i_j}).$$

Note, in particular, two events E and F are independent if

$$P(E \cap F) = P(E)P(F)$$

Example 4.7.2. **Aircraft safety.**

An aircraft safety system contains n independent components. The aircraft can fly provided at least one of the components is working. The probability that the ith component works is p_i. Then

$$\begin{aligned} P(\text{Aircraft can fly}) &= 1 - P(\text{Aircraft cannot fly}) \\ &= 1 - P(\text{All components fail}) \\ &= 1 - \prod_{i=1}^{n} P(\text{Component } i \text{ fails}) \\ &= 1 - \prod_{i=1}^{n} (1 - p_i). \end{aligned}$$

Task: Session 3

Attempt the **R Markdown** file for Session 3:
Session 3: Probability in R

Student Exercises

Attempt the exercises below.

Exercise 4.1.
A card is drawn from a standard pack of 52. Let B be the event 'the card is black', NA the event 'the card is not an Ace' and H the event 'the card is a Heart'. Calculate the following probabilities:

(a) $P(B|NA)$;

(b) $P(NA|B^c)$;

(c) $P(B^c \cap H|NA)$;

(d) $P(NA \cup B|H^c)$;

(e) $P(NA \cup H|NA \cap B)$.

Exercise 4.2.
A diagnostic test has a probability 0.95 of giving a positive result when applied to a person suffering from a certain disease, and a probability 0.10 of giving a (false) positive when applied to a non-sufferer. It is estimated that 0.5% of the population are sufferers. Suppose that the test is applied to a person chosen at random from the population. Find the probabilities of the following events.

(a) the test result will be positive.

(b) the person is a sufferer, given a positive result.

(c) the person is a non-sufferer, given a negative result.

(d) the person is missclassified.

Exercise 4.3.
In areas such as market research, medical research, etc, it is often hard to get people to answer embarrassing questions. One way around this is the following. Suppose that N people are interviewed, where N is even. Each person is given a card, chosen at random from N cards, containing a single question. Half of the cards contain the embarrassing question, to which the answer is either 'Yes' or 'No'. The other half of the cards contain the question 'Is your birthday between January and June inclusive?'

Suppose that of the N people interviewed, R answer 'Yes' to the question that they received. Let Y be the event that a person gives a 'Yes' answer, E the event that they received a card asking the embarrassing question. Assuming that half the population have birthdays between January and June inclusive, write down:

(a) $P(Y)$;

(b) $P(E)$;

(c) $P(Y|E^c)$.

Hence calculate the proportion of people who answered 'Yes' to the embarrassing question.

Hint: Try writing down an expression for $P(Y)$ using the Theorem of Total

Probability.

Comment on your answer.

Chapter 5

Random Variables

5.1 Overview

In this Chapter we will introduce the concept of a **random variable** (Section 5.2). Random variables assign numerical values to outcomes from a sample space and these can be discrete (counts), continuous (measurements on the real-line) or mixed. Key summaries for random variables are their expectation (mean) and variance, concepts that we have already seen for summarising data and which in Section 5.3 we formalise for random variables. We introduce important classes of random variables (probability distributions), both discrete and continuous distributions. These include:

- Section 5.4 Bernoulli random variables and their extensions such as the Bernoulli, Binomial, Geometric and Negative Binomial distributions
- Section 5.5 Poisson distribution
- Section 5.6 Exponential random variables and their extensions such as the Exponential, Gamma, Chi-squared and Beta distributions
- Section 5.7 Normal (Gaussian) distribution

5.2 Random variables

Definition 5.2.1. **Random variable.**

A *random variable* (r.v.) X is a mapping from Ω to $\mathbb{R}$, that is

$$X : \Omega \longrightarrow \mathbb{R}.$$

For example,

- Let X be the number of heads observed when tossing a fair coin three times.
- Let T be the length of time you wait to be serviced by a bank teller.

Note: Random variables can be either discrete (*i.e.* take a finite or countable number of values), continuous, or mixed.

An example of a mixed random variable is, R, the amount of rain (ml) on a given day.

Definition 5.2.2. **Cumulative distribution function.**

The *cumulative distribution function* (c.d.f.) of a random variable X is

$$F_X(x) = P(X \leq x) = P(\{\omega \in \Omega : X(\omega) \leq x\}).$$

Properties of the c.d.f include

- $P(X > x) = 1 - F_X(x)$.
- $P(x_1 < X \leq x_2) = F_X(x_2) - F_X(x_1)$.

Note the c.d.f. is defined for all random variables regardless of whether they are discrete, continuous or mixed.

Definition 5.2.3. **Probability mass function.**

If X is a **discrete** random variable, then we can define a function $p_X(x)$, called the *probability mass function* (p.m.f.) such that

$$p_X(x_i) = P(X = x_i) = P(\{\omega : X(\omega) = x_i\}).$$

Example 5.2.4. **Coin toss.**

Let X be the number of heads observed when tossing a fair coin three times. What is the p.m.f. of X?

$$p_X(x) = \begin{cases} 1/8, & \text{if } x = 0, \\ 3/8, & \text{if } x = 1, \\ 3/8, & \text{if } x = 2, \\ 1/8, & \text{if } x = 3, \\ 0, & \text{otherwise.} \end{cases}$$

Definition 5.2.5. **Probability density function.**

Let X be a **continuous** random variable. If there exists some non-negative function f_X on $\mathbb{R}$ such that for any interval I,

$$P(X \in I) = \int_I f_X(u)du,$$

the function f_X is called the *probability density function* (p.d.f.) of X.

Note that if $F_X(x)$ is the c.d.f. of a continuous random variable X, then the p.d.f. of X is given by

$$f_X(x) = \frac{dF_X(x)}{dx}.$$

Note that

$$F_X(x) = P(X \leq x) = \begin{cases} \sum\limits_{x_i \leq x} p_X(x_i), & \text{if } X \text{ is discrete,} \\ \int_{-\infty}^{x} f_X(u)du, & \text{if } X \text{ is continuous.} \end{cases}$$

5.3 Expectation

In this Section we formally define the expectation (mean), variance, median and mode of a random variable. We can note the similarities with the definitions of the measures of location (mean, median and mode) and variance of summary statistics in Section 2.

Definition 5.3.1. **Expectation.**

The *expectation* of a random variable X is defined by

$$E[X] = \begin{cases} \sum\limits_{x_i} x_i p_X(x_i), & \text{if } X \text{ is discrete,} \\ \int_{-\infty}^{\infty} x f_X(x)dx, & \text{if } X \text{ is continuous.} \end{cases}$$

Note that $E[X]$ only exists if $E[|X|] < \infty$ and that $E[X]$ is a measure of the *centre* of the distribution, that is the centre of mass. We can also define expectations of functions of random variables.

Definition 5.3.2.
If $Y = g(X)$ then the *expectation* of Y is given by

$$E[Y] = E[g(X)] \qquad = \begin{cases} \sum_{x_i} g(x_i) p_X(x_i), & \text{if } X \text{ is discrete,} \\ \int_{-\infty}^{\infty} g(x) f_X(x)\, dx, & \text{if } X \text{ is continuous.} \end{cases}$$

For constants c, c_i and d, the following are properties of the expectation:

- $E[c] = c$;
- $E[cg(X) + d] = cE[g(X)] + d$;
- $E\left[\sum_{i=1}^{n} c_i g_i(X_i)\right] = \sum_{i=1}^{n} c_i E[g_i(X_i)]$;
- A special case of the above results is $c_1 = ... = c_n = 1$ and $g_i(\cdot)$ is the identity transform, $g_i(X_i) = X_i$. Then $E\left[\sum_{i=1}^{n} X_i\right] = \sum_{i=1}^{n} E[X_i]$.

Definition 5.3.3. **Variance.**

The *variance* of X is

$$\text{Var}(X) = E\left[(X - E[X])^2\right].$$

The *standard deviation* of X is $\sqrt{\text{Var}(X)}$.

For constants c, c_i and d, the following are properties of the variance:

- $\text{Var}(X) = E[X^2] - (E[X])^2$;
- $\text{Var}(X) \geq 0$;
- $\text{Var}(cX + d) = c^2 \text{Var}(X)$;
- If $X_1, ..., X_n$ are independent, then

$$\text{Var}\left(\sum_{i=1}^{n} c_i X_i\right) = \sum_{i=1}^{n} c_i^2 \text{Var}(X_i).$$

Definition 5.3.4. **Median.**

The *median* of X is defined as x_0 such that $F_X(x_0) = 0.5$.

For a discrete random variable it is unlikely that there exists x_0 such that $F_X(x_0) = 0.5$. Therefore for discrete random variables the median is defined to be the smallest x_0 such that $F_X(x_0) \geq 0.5$.

Definition 5.3.5. **Mode.**

The *mode* of X is the point at which $f_X(x)$ is maximised, *i.e.* mode is x_0 if and only if $f_X(x_0) \geq f_X(x)$ for all x.

Example 5.3.6. **Continuous distribution.**

Suppose that the random variable X has probability density function:

$$f_X(x) = \begin{cases} kx^3 & 1 \leq x \leq 2, \\ 0 & \text{otherwise.} \end{cases}$$

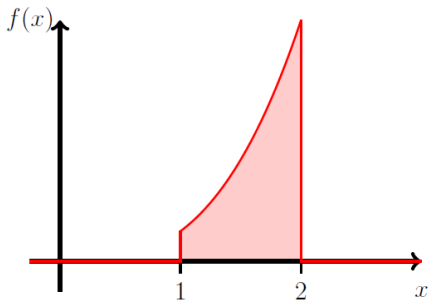


Figure 5.1: Plot of $f_X(x)$.

1. Show that $k = 4/15$;

2. Find $P(\frac{5}{4} \leq X \leq \frac{7}{4})$.
3. Compute the standard deviation of X.
   Remember: Standard deviation is the square root of the variance.

4. Find the median of X.

Attempt Example 5.3.6 and then watch Video 10 for the solutions.

Watch Video 10: Continuous random variable

Solution to Example 5.3.6.

1. Remember $\int_{-\infty}^{\infty} f_X(x)\,dx = 1$ and therefore

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} f_X(x)\,dx \\ &= \int_1^2 kx^3\,dx \\ &= k\left[\frac{x^4}{4}\right]_1^2 \\ &= k\left(\frac{2^4}{4} - \frac{1^4}{4}\right) = k \times \frac{15}{4}. \end{aligned}$$

Thus, $k = \frac{4}{15}$.

2. It follows from the above that the c.d.f of X is

$$F_X(x) = \begin{cases} 0 & \text{for } x < 1 \\ \int_1^x \frac{4}{15} y^3\,dy = \frac{x^4-1}{15} & \text{for } 1 \le x \le 2 \\ 1 & \text{for } x > 2 \end{cases}$$

Thus

$$\begin{aligned} P\left(\frac{5}{4} \le X \le \frac{7}{4}\right) &= \frac{(7/4)^4 - 1}{15} - \frac{(5/4)^4 - 1}{15} \\ &= \frac{1}{15}\left[\left(\frac{7}{4}\right)^4 - \left(\frac{5}{4}\right)^4\right] \\ &= \frac{37}{80} (= 0.4625). \end{aligned}$$

3. Remember that the standard deviation of X is the square root of the variance. Therefore

$$sd(X) = \sqrt{var(X)} = \sqrt{E[X^2] - E[X]^2}.$$

For any $n = 1, 2, ...,$

$$\begin{aligned} E[X^n] &= \int_{-\infty}^{\infty} x^n f_X(x)\,dx \\ &= \int_1^2 x^n \frac{4}{15}x^3\,dx \\ &= \frac{4}{15}\left[\frac{x^{n+4}}{n+4}\right]_1^2 \\ &= \frac{4(2^{n+4}-1)}{15(n+4)}. \end{aligned}$$

Therefore

$$\begin{aligned} E[X] &= \frac{4(32-1)}{15\times 5} = \frac{124}{75} = 1.6533 \\ E[X^2] &= \frac{4(64-1)}{15\times 6} = \frac{14}{5} = 2.8 \end{aligned}$$

Thus

$$sd(X) = \sqrt{2.8 - 1.6533^2} = 0.2579.$$

4. The median of X, m, satisfies

$$\begin{aligned} 0.5 &= P(X \le m) = \frac{m^4-1}{15} \\ 7.5 &= m^4 - 1 \\ 8.5 &= m^4. \end{aligned}$$

Therefore

$$m = (8.5)^{1/4} = 1.7075.$$

5.4 Bernoulli distribution and its extension

In this section, we start with the Bernoulli random variable, which is the simplest non-trivial probability distribution taking two possible values (0 or 1). In itself the Bernoulli random variable might not seem particularly exciting, but it forms a key building block in probability and statistics. We consider probability distributions which arise as extensions of the Bernoulli random variable such as the Binomial distribution (sum of n Bernoulli random variables), the Geometric distribution (number of Bernoulli random variables until we get a 1) and the Negative Binomial distribution (number of Bernoulli random variables until we get our n^{th} 1).

5.4.1 Bernoulli distribution

Definition 5.4.1. **Bernoulli trial.**

A *Bernoulli trial* is a simple random experiment with two outcomes: success (1) or failure (0). The success probability is p, so failure probability $= 1 - p(= q)$. A Bernoulli random variable X describes this:

$$X = \begin{cases} 1 & \text{success - probability } p, \\ 0 & \text{failure - probability } q = 1 - p. \end{cases}$$

The Bernoulli distribution has probability mass function:

$$p_X(x) = p^x(1-p)^{1-x} \qquad x = 0, 1.$$

[If $x = 1$, $p_X(1) = p^1 q^0 = p$ and if $x = 0$, $p_X(0) = p^0 q^1 = q$.]

We have that

$$E[X] = [p \times 1] + [q \times 0] = p$$

and

$$E[X^2] = [p \times 1^2] + [q \times 0^2] = p.$$

Therefore

$$var(X) = E[X^2] - E[X]^2 = p - p^2 = p(1-p) = pq.$$

5.4.2 Binomial Distribution

Definition 5.4.2. **Independent and identically distributed**
Two discrete random variables X and Y are said to be **independent and identically distributed** (*i.i.d.*) if for all $x, y \in \mathbb{R}$,

$$P(X = x, Y = y) = P(X = x) \times P(Y = y) \quad \text{(independence)}$$

and for all $x \in \mathbb{R}$,

$$P(Y = x) = P(X = x),$$

(identically distributed, *i.e.* have the same pmf.)

Definition 5.4.3. **Binomial distribution.**

Consider n independent Bernoulli trials, each with success probability p. Let X be the total number of successes. Then X has a *Binomial* distribution, written

$$X \sim \text{Bin}(n, p), \quad \text{or } X \sim \text{B}(n, p)$$

and for $k = 0, 1, \ldots, n$,

$$p_X(k) = P(X = k) = \binom{n}{k} p^k (1-p)^{n-k}.$$

To see this: consider any particular sequence of k successes and $n - k$ failures. Each such sequence has probability $p^k(1-p)^{n-k}$, since the n trials are independent. There are $\binom{n}{k}$ ways of choosing the positions of the k successes out of n trials.

Note: 1. n and p are called the parameters of the Binomial distribution.
2. The number of trials n is fixed.
3. There are only two possible outcomes: 'success' with probability p and 'failure' with probability $q = 1 - p$.
4. The probability of success p in each independent trial is constant.

Lemma 5.4.4. **Binomial distribution: Expectation and variance.**

Let $X \sim \text{Bin}(n, p)$, then

$$E[X] = np \quad \text{and} \quad var(X) = np(1-p).$$

We can write

$$X = X_1 + X_2 + ... + X_n, \tag{5.1}$$

where $X_1, X_2, ..., X_n$ are independent Bernoulli random variables each with success probability p.

Therefore using properties of expectations

$$\begin{aligned} E[X] &= E[X_1 + X_2 + ... + X_n] \\ &= E[X_1] + E[X_2] + ... + E[X_n] \\ &= p + p + ... + p = np. \end{aligned}$$

Given that the X_i's in (5.1) are independent, we also have that

$$\begin{aligned} var(X) &= var(X_1 + X_2 + ... + X_n) \\ &= var(X_1) + var(X_2) + ... + var(X_n) \\ &= p(1-p) + p(1-p) + ... + p(1-p) = np(1-p). \end{aligned}$$

The cumulative distribution function is

$$F_X(x) = P(X \leq x) = \sum_{k=0}^{[x]} \binom{n}{k} p^k (1-p)^{n-k},$$

where $[x]$ is the greatest integer not greater than x.

An **R Shiny** app is provided to explore the Binomial distribution.

R Shiny app: Binomial distribution

Example 5.4.5.
Twenty multiple choice questions, each with 5 options. Suppose that you guess at random, independently for each question. Then if X is the number of right

answers,

$$X \sim Bin(20, 0.2).$$

Then

$$P(X = 3) = \binom{20}{3}(0.2)^3(0.8)^{17} = 0.2053,$$

and

$$P(X \leq 3) = \sum_{k=0}^{3}\binom{20}{k}(0.2)^k(0.8)^{20-k} = 0.4114.$$

5.4.3 Geometric Distribution

Definition 5.4.6. **Geometric distribution.**

Consider a sequence of independent Bernoulli trials each with success probability p. Let Y denote the number of trials needed for the first success to appear. Then Y has a *Geometric* distribution with parameter p, written $Y \sim Geom(p)$, and

$$p_Y(k) = (1-p)^{k-1}p, \quad k = 1, 2, 3, \ldots.$$

To see this: If the k^{th} trial is the first success then the first $k-1$ trials must have been failures. Probability of this is $(1-p)^{k-1}p$.

Note that

$$\sum_{k=1}^{\infty} p_Y(k) = \sum_{k=1}^{\infty}(1-p)^{k-1}p = p\sum_{i=0}^{\infty}(1-p)^i = \frac{p}{1-(1-p)} = 1,$$

so a success eventually occurs with probability 1.

Lemma 5.4.7. **Geometric distribution: Expectation and variance.**

Let $Y \sim \text{Geom}(p)$, then

$$E[Y] = \frac{1}{p} \quad \text{and} \quad var(Y) = \frac{1-p}{p^2}.$$

First step: Let $q = 1 - p$ and write

$$\begin{aligned} E[Y] &= \sum_{k=1}^{\infty} kP(Y = k) \\ &= \sum_{k=1}^{\infty} k(1-p)^{k-1}p \\ &= p\sum_{k=1}^{\infty} kq^{k-1} \end{aligned}$$

Note that kq^{k-1} is the derivative of q^k with respect to q. Hence,

$$E[Y] = p\sum_{k=1}^{\infty} \frac{\mathrm{d}}{\mathrm{d}q}\left\{q^k\right\}.$$

We can interchange the order of summation and differentiation (we won't go into the technical requirements):

$$\begin{aligned} E[Y] &= p\frac{\mathrm{d}}{\mathrm{d}q}\left(\sum_{k=1}^{\infty} q^k\right) \\ &= p\frac{\mathrm{d}}{\mathrm{d}q}\left(\frac{q}{1-q}\right), \end{aligned}$$

since $\sum_{k=1}^{\infty} x^k = x/(1-x)$ if $|x| < 1$.

Therefore

$$\begin{aligned} E[Y] &= p\frac{(1)(1-q) - q(-1)}{(1-q)^2} \\ &= \frac{p}{p^2} = \frac{1}{p}. \end{aligned}$$

By a similar method, we obtain

$$E[Y(Y-1)] = \frac{2(1-p)}{p^2}.$$

Since

$$E[Y(Y-1)] = E[Y^2 - Y] = E[Y^2] - E[Y], \tag{5.2}$$

we have that

$$var(Y) = E[Y(Y-1)] + E[Y] - E[Y]^2 = \frac{1-p}{p^2}.$$

5.4.4 Negative binomial Distribution

Definition 5.4.8. **Negative binomial distribution.**

Consider a sequence of independent Bernoulli trials, each with success probability p. If W is the number of trials needed until r successes have occurred then W has a *Negative Binomial* distribution, $W \sim \text{NegBin}(r, p)$, with probability mass function

$$p_W(k) = \binom{k-1}{r-1} p^r (1-p)^{k-r} \quad k = r, r+1, ...$$

To see this: We must have the k^{th} trial is successful and that it is the r^{th} success. Therefore we have $r-1$ successes in first $k-1$ trials, the locations of which can be chosen in $\binom{k-1}{r-1}$ ways.

Lemma 5.4.9. **Negative binomial distribution: Expectation and variance.**

Let $W \sim \text{NegBin}(r, p)$, then

$$E[W] = \frac{r}{p} \quad \text{and} \quad var(W) = \frac{r(1-p)}{p^2}.$$

Note that we can write

$$W = Y_1 + Y_2 + ... + Y_r,$$

where Y_1 is the number of trials until the first success and, for $i = 2, 3, ..., r$, Y_i is the number of trials after the $(i-1)^{st}$ success until the i^{th} success.

We observe that $Y_1, Y_2, ..., Y_r$ are independent $\text{Geom}(p)$ random variables, so

$$E[Y_1] = \frac{1}{p} \quad \text{and} \quad var(Y_1) = \frac{1-p}{p^2},$$

whence

$$E[W] = E[Y_1 + Y_2 + ... + Y_r] = E[Y_1] + E[Y_2] + ... + E[Y_r] = \frac{r}{p},$$

and

$$var(W) = var(Y_1 + Y_2 + ... + Y_r) = var(Y_1) + var(Y_2) + ... + var(Y_r) = \frac{r(1-p)}{p^2}.$$

The negative binomial distribution $W \sim \text{NegBin}(r, p)$ is the sum of r independent geometric, $Y \sim \text{Geom}(p)$ distributions in the same way that the binomial distribution $X \sim \text{Bin}(n, p)$ is the sum of n independent Bernoulli random variables with success probability p.

An **R Shiny** app is provided to explore the Negative Binomial distribution.

R Shiny app: Negative Binomial distribution

Example 5.4.10 draws together the different Bernoulli-based distributions and demonstrates how they are used to answer different questions of interest.

Example 5.4.10. **Crazy golf.**

Figure 5.2: Crazy golf picture.

A child plays a round of crazy golf. The round of golf consists of 9 holes. The number of shots the child takes at each hole is geometrically distributed with success probability 0.25.

(a) Calculate the probability that the child gets a 'hole in one' on the first hole. (A 'hole in one' means the child only takes one shot on that hole.)

(b) Calculate the probability that the child takes more than five shots on the first hole.

(c) Calculate the probability that the child gets three 'hole in one' during their round.

(d) Calculate the mean and variance for the total number of shots the child takes.

(e) Calculate the probability that the child takes 36 shots in completing their round.

Attempt Example 5.4.10 (Crazy golf) and then watch Video 11 for the solutions.

Watch Video 11: Crazy Golf Example

Solution to Example 5.4.10.

Let X_i denote the number of shots taken on hole i. Then $X_i \sim \text{Geom}(0.25)$.

(a) A 'hole in one' on the first hole is the event $\{X_1 = 1\}$. Therefore

$$P(\text{Hole in one}) = P(X_1 = 1) = 0.25.$$

(b) More than five shots on the first hole is the event $\{X_1 > 5\}$. Therefore

$$P(X_1 > 5) = 0.75^5 = 0.2373.$$

(c) This is a binomial question since there are $n = 9$ holes and on each hole there is $p = P(X_1 = 1) = 0.25$ of obtaining a hole in one. Let $Y \sim \text{Bin}(9, 0.25)$ denote the number of holes in one in a round, then

$$P(Y = 3) = \binom{9}{3}(0.25)^3(0.75)^6 = 0.2336.$$

(d) The total number of shots taken is

$$Z = X_1 + X_2 + ... + X_9 \sim \text{NegBin}(9, 0.25).$$

Thus the mean number of shots taken is $E[Z] = \frac{9}{0.25} = 36$ and the variance of the number of shots is $var(Z) = \frac{9(1-0.25)}{0.25^2} = 108$.

(e) The probability that the child takes exactly 36 (mean number of) shots is

$$P(Z = 36) = \binom{36-1}{9-1}(0.25)^9(0.75)^{27} = 0.0380.$$

5.5 Poisson distribution

The Poisson distribution is often used to model 'random' events - *e.g.* hits on a website; traffic accidents; customers joining a queue etc.

Suppose that events occur at rate $\lambda > 0$ per unit time. Divide the time interval $[0, 1)$ into n small equal parts of length $1/n$.

$$[0,1) = \left[0, \frac{1}{n}\right) \cup \left[\frac{1}{n}, \frac{2}{n}\right) \cup ... \cup \left[\frac{i}{n}, \frac{i+1}{n}\right) \cup ... \cup \left[\frac{n-1}{n}, 1\right).$$

Assume that each interval can have either zero or one event, independently of other intervals, and

$$P\left[1 \text{ event in } \left[\frac{i}{n}, \frac{i+1}{n}\right)\right] = \frac{\lambda}{n}.$$

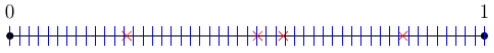


Figure 5.3: Four events (red crosses) in 50 sub-intervals of [0,1].

Let X be the number of events in the time interval $[0, 1)$. Then

$$X \sim \text{Bin}(n, \lambda/n)$$

and letting $n \to \infty$, (the number of intervals grows but the chance of observing an event in a given interval decreases), we have that

$$\begin{aligned}
P(X = k) &= \binom{n}{k} \left(\frac{\lambda}{n}\right)^k \left(1 - \frac{\lambda}{n}\right)^{n-k} \\
&= \frac{n(n-1)\ldots(n-k+1)}{k!} \times \frac{\lambda^k}{n^k} \times \left(1 - \frac{\lambda}{n}\right)^{n-k} \\
&= \frac{n(n-1)\ldots(n-k+1)}{n^k} \times \frac{\lambda^k}{k!} \times \frac{(1-\lambda/n)^n}{(1-\lambda/n)^k} \\
&= 1\left(1 - \frac{1}{n}\right)\cdots\left(1 - \frac{(k-1)}{n}\right) \times \frac{\lambda^k}{k!} \times \frac{(1-\lambda/n)^n}{(1-\lambda/n)^k} \\
&\to 1 \times \frac{\lambda^k}{k!} \times \exp(-\lambda) \quad \text{as } n \to \infty, \text{ for fixed } k.
\end{aligned}$$

Definition 5.5.1. **Poisson distribution**

Let X be a **discrete** random variable with parameter $\lambda > 0$ and p.m.f.

$$P(X = x) = \frac{\lambda^x}{x!} \exp(-\lambda) \qquad (x = 0, 1, \ldots).$$

Then X is said to follow a **Poisson** distribution with parameter λ, denoted $X \sim \text{Po}(\lambda)$.

Lemma 5.5.2. **Poisson distribution: Expectation and variance.**

Let $X \sim \text{Po}(\lambda)$, then

$$E[X] = \lambda \quad \text{and} \quad var(X) = \lambda.$$

By definition of expectation,

$$E[X] = \sum_{x=0}^{\infty} xP(X = x) = \sum_{x=1}^{\infty} xP(X = x),$$

since $0 \times P(X = 0) = 0$.

Now

$$\begin{aligned} E[X] &= \sum_{x=1}^{\infty} x \times \frac{\lambda^x}{x!} \exp(-\lambda) \\ &= \exp(-\lambda) \sum_{x=1}^{\infty} \frac{x\lambda^x}{x!} = \lambda \exp(-\lambda) \sum_{x=1}^{\infty} \frac{\lambda^{x-1}}{(x-1)!}. \end{aligned}$$

Using a change of variable $k = x - 1$,

$$E[X] = \lambda \exp(-\lambda) \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} = \lambda \exp(-\lambda) \exp(\lambda) = \lambda.$$

Similarly, we can show that

$$E[X(X-1)] = \sum_{x=0}^{\infty} x(x-1) \left(\frac{\lambda^x}{x!} \exp(-\lambda) \right) = \lambda^2.$$

Therefore, as noted in Lemma 5.4.7 (5.2), we have that $E[X^2] = E[X(X-1)] + E[X]$ giving

$$\begin{aligned} var(X) &= E[X(X-1)] + E[X] - E[X]^2 \\ &= \lambda^2 + \lambda - \lambda^2 = \lambda. \end{aligned}$$

5.6 Exponential distribution and its extensions

In this section we start with the Exponential random variable which is an important continuous distribution that can take positive values (on the range $[0, \infty)$). The Exponential distribution is the continuous analogue of the Geometric distribution. The sum of exponential distributions leads to the Erlang distribution which is a special case of the Gamma distribution. Another special case of the

Gamma distribution is the χ^2 (Chi squared) distribution which is important in statistics. Finally, we consider the Beta distribution which is continuous distribution taking values on the range $(0, 1)$ and can be constructed from Gamma random variables via a transformation. (See Section 14 for details on transformations.)

5.6.1 Exponential distribution

Let X denote the total number of hits on a website in time t. Let λ - rate of hits per unit time, and so, λt - rate of hits per time t.

A suitable model as we have observed in Section 5.5 for X is $\text{Po}(\lambda t)$.

Let T denote the time, from a fixed point, until the first hit. Note that T is continuous $0 < T < \infty$ whilst the number of hits X is discrete. Then $T > t$ if and only if $X = 0$. Hence,

$$P(T > t) = P(X = 0) = \exp(-\lambda t)$$

and so,

$$P(T \leq t) = 1 - \exp(-\lambda t) \quad (t > 0).$$

Therefore the cumulative distribution function of T is

$$F_T(t) = \begin{cases} 0 & t < 0 \\ 1 - \exp(-\lambda t) & t \geq 0 \end{cases}$$

Differentiating $F_T(t)$ with respect to t gives

$$f_T(t) = \begin{cases} 0 & t < 0 \\ \lambda \exp(-\lambda t) & t \geq 0 \end{cases}$$

Definition 5.6.1. **Exponential distribution**

A random variable T is said to have an exponential distribution with parameter $\lambda > 0$, written $T \sim \text{Exp}(\lambda)$ if its c.d.f. is given by

$$F_T(t) = \begin{cases} 1 - e^{-\lambda t} & t > 0 \\ 0 & t \leq 0, \end{cases}$$

and its p.d.f. is

$$f_T(t) = \frac{d}{dt} F_T(t) = \begin{cases} \lambda e^{-\lambda t} & t > 0 \\ 0 & t \leq 0 \end{cases}$$

Lemma 5.6.2. **Exponential distribution: Expectation and variance.**

Let $T \sim \text{Exp}(\lambda)$, then

$$E[T] = \frac{1}{\lambda} \quad \text{and} \quad var(T) = \frac{1}{\lambda^2}.$$

The expectation of T is

$$E[T] = \int_{-\infty}^{\infty} t f_T(t)\, dt = \int_0^{\infty} t\lambda e^{-\lambda t}\, dt.$$

Using integration by parts, we have that

$$\begin{aligned} E[T] &= [t \times -e^{-\lambda t}]_0^{\infty} - \int_0^{\infty} -e^{-\lambda t}\, dt \\ &= (0-0) + \left[-\frac{1}{\lambda} e^{-\lambda t}\right]_0^{\infty} = \frac{1}{\lambda}. \end{aligned}$$

Similarly, by using integration parts twice,

$$E[T^2] = \int_0^{\infty} t^2 \lambda e^{-\lambda t}\, dx = \frac{2}{\lambda^2}.$$

Therefore the variance of T is

$$var(T) = E[T^2] - E[T]^2 = \frac{2}{\lambda^2} - \frac{1}{\lambda^2} = \frac{1}{\lambda^2}.$$

5.6.2 Gamma distribution

Suppose that we want to know, W, the time until the m^{th} $(m = 1, 2, ...)$ hit on a website. Then

$$W = T_1 + T_2 + ... + T_m$$

where T_i is the time from the $(i-1)^{st}$ hit on the website until the i^{th} hit on the website.

Note that $T_1, T_2, ...$ are independent and identically distributed i.i.d. according to $T \sim \text{Exp}(\lambda)$. That is, W is the sum of m exponential random variables with parameter λ. Then W follows a Gamma distribution with $W \sim \text{Gamma}(m, \lambda)$.

Definition 5.6.3. **Gamma distribution**

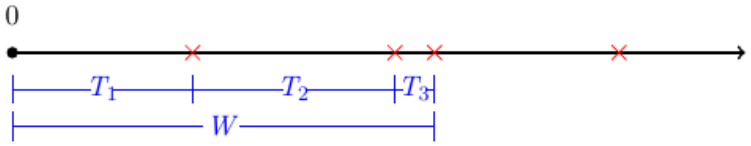


Figure 5.4: Illustration with $m = 3$, $W = T_1 + T_2 + T_3$.

A random variable X is said to have a Gamma distribution with parameters $\alpha, \beta > 0$, written $X \sim \text{Gamma}(\alpha, \beta)$ if its p.d.f. is given by

$$f_X(x) = \begin{cases} \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} \exp(-\beta x) & x > 0 \\ 0 & x \leq 0, \end{cases}$$

where $\Gamma(\alpha) = \int_0^\infty y^{\alpha-1} \exp(-y)\, dy$.

Note that if α is an integer $\Gamma(\alpha) = (\alpha - 1)!$. Also $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$ and for $\alpha > 1$,

$$\Gamma(\alpha) = (\alpha - 1)\Gamma(\alpha - 1).$$

By definition, for $\alpha = 1$, $X \sim \text{Exp}(\beta)$ and for $\alpha \in \mathbb{N}$, the Gamma distribution is given by the sum of α exponential random variables. The special case where α is integer is sometimes referred to as the **Erlang distribution**. However, the gamma distribution is defined for positive, real-valued α.

The α parameter is known as the *shape* parameter and determines the shape of the Gamma distribution. In particular, the shape varies dependent on whether $\alpha < 1$, $\alpha = 1$ or $\alpha > 1$.

- $\alpha < 1$, the modal value of X is at 0 and $f(x) \to \infty$ as $x \downarrow 0$ (x tends to 0 from above).
- $\alpha = 1$, the exponential distribution. The modal value of of X is at 0 and $f(0) = \beta$.
- $\alpha > 1$, $f(0) = 0$ and the modal value of X is at $\frac{\alpha-1}{\beta}$.

The β parameter is known as the *scale* parameter. It does not affect the shape of the Gamma distribution but has the property that if $U \sim \text{Gamma}(\alpha, 1)$, then X has the same distribution as U/β. This can be written as

$$X \stackrel{D}{=} \frac{U}{\beta} \sim \frac{1}{\beta}\text{Gamma}(\alpha, 1).$$

Definition 5.6.4. **Equality in distribution**

Two random variables X and Y are said to be *equal in distribution*, denoted $X \overset{D}{=} Y$, if for all $x \in \mathbb{R}$,

$$P(X \leq x) = P(Y \leq x).$$

That is, X and Y have the same c.d.f., or equivalently, X and Y have the same p.d.f. (p.m.f.) if X and Y are continuous (discrete).

An **R Shiny** app is provided to explore the Gamma distribution.

R Shiny app: Gamma distribution

Lemma 5.6.5. **Gamma distribution: Expectation and variance.**

If $X \sim \text{Gamma}(\alpha, \beta)$ then

$$E[X] = \frac{\alpha}{\beta}, \quad var(X) = \frac{\alpha}{\beta^2}.$$

The proof is straightforward if $\alpha = m \in \mathbb{N}$ since then $X = T_1 + T_2 + ... + T_m$, where the T_i are *i.i.d.* according to $T \sim \text{Exp}(\beta)$. (Compare with the proof of Lemma 5.4.9 for the mean and variance of the negative binomial distribution.)

We omit the general proof for $\alpha \in \mathbb{R}^+$, which can be proved by integration by parts.

We have noted that the Gamma distribution arises as the sum of exponential distributions. More general if $X_1 \sim \text{Gamma}(\alpha_1, \beta)$ and $X_2 \sim \text{Gamma}(\alpha_2, \beta)$ are independent gamma random variables with a common scale parameter $\beta > 0$, then

$$X_1 + X_2 \sim \text{Gamma}(\alpha_1 + \alpha_2, \beta).$$

5.6.3 Chi squared distribution

The chi squared (χ^2) distribution is a special case of the Gamma distribution which plays an important role in statistics. For $k \in \mathbb{N}$, if

$$X \sim \text{Gamma}\left(\frac{k}{2}, \frac{1}{2}\right)$$

then X is said to follow a chi squared distribution with k degrees of freedom. Note that X has probability density function

$$f_X(x) = \begin{cases} \frac{x^{\frac{k}{2}-1}\exp(-\frac{x}{2})}{2^{\frac{k}{2}}\Gamma(\frac{k}{2})} & x > 0 \\ 0 & x \leq 0, \end{cases}$$

with $E[X] = k$ and $var(X) = 2k$.

5.6.4 Beta distribution

Suppose that X and Y are **independent** random variables such that $X \sim \text{Gamma}(\alpha, \gamma)$ and $Y \sim \text{Gamma}(\beta, \gamma)$ for some $\alpha, \beta, \gamma > 0$. Note that both X and Y have the same scale parameter γ. Let

$$Z = \frac{X}{X+Y},$$

the proportion of the sum of X and Y accounted for by X. Then Z will take values on the range $[0, 1]$ and Z follows a Beta distribution with parameters α and β.

Lemma 5.6.6. **Beta distribution**

A random variable Z is said to have a Beta distribution with parameters $\alpha, \beta > 0$, written $Z \sim \text{Beta}(\alpha, \beta)$ if its pdf is given by

$$f_Z(z) = \begin{cases} \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} z^{\alpha-1}(1-z)^{\beta-1} & 0 < z < 1 \\ 0 & \text{otherwise.} \end{cases}$$

Note that if $Z \sim \text{Beta}(\alpha, \beta)$, then

$$E[Z] = \frac{\alpha}{\alpha+\beta} \quad \text{and} \quad var(Z) = \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}.$$

The special case where $\alpha = \beta = 1$, $f_Z(z) = 1$ $(0 < z < 1)$ and Z is uniformly distributed on $[0, 1]$ denoted $Z \sim U(0, 1)$. That is,

$$\text{Beta}(1, 1) \stackrel{D}{=} U(0, 1).$$

An **R Shiny** app is provided to explore the Beta distribution.

R Shiny app: Beta distribution

Example 5.6.7 (Catching a bus) draws together the different Exponential-based distributions and demonstrates how they are used to answer different questions of interest.

Example 5.6.7. **Catching a bus.**

Suppose that the time (in minutes) between buses arriving at a bus stop follows an Exponential distribution, $Y \sim \text{Exp}(0.5)$. Given you arrive at the bus stop just as one bus departs:

Figure 5.5: Bus picture.

(a) Calculate the probability that you have to wait more than 2 minutes for the bus.

(b) Calculate the probability that you have to wait more than 5 minutes for the bus given that you wait more than 3 minutes.

(c) Given that the next two buses are full, what is the probability you have to wait more than 6 minutes for a bus (the third bus to arrive)?

(d) What is the probability that the time until the third bus arrives is more than double the time until the second bus arrives?

Attempt Example 5.6.7 (Catching a bus) and then watch Video 12 for the solutions.

Watch Video 12: Catching a bus

Solution to Example 5.6.7.

For an exponential random variable, $X \sim \text{Exp}(\beta)$, we have that for any $x > 0$,

$$P(X > x) = 1 - P(X \leq x) = 1 - \{1 - \exp(-\beta x)\} = \exp(-\beta x).$$

(a) Since $Y \sim \text{Exp}(0.5)$,

$$P(Y > 2) = \exp(-0.5(2)) = \exp(-1) = 0.3679.$$

(b) Note that $\{Y > 5\}$ implies that $\{Y > 3\}$. Therefore

$$P(Y > 5|Y > 3) = \frac{P(Y > 5)}{P(Y > 3)} = \frac{\exp(-0.5(5))}{\exp(-0.5(3))} = \exp(-1) = 0.3679.$$

Therefore

$$P(Y > 5|Y > 3) = P(Y > 2).$$

This property is known as the **memoryless** property of the exponential distribution, for any $s, t > 0$,

$$P(Y > s + t|Y > s) = P(Y > t).$$

(c) The time, W, until the third bus arrives is $W \sim \text{Gamma}(3, 0.5)$. Therefore

$$f_W(w) = \frac{0.5^3}{(3-1)!} w^{3-1} \exp(-0.5w) \qquad (w > 0),$$

and

$$F_W(w) = 1 - \exp(-0.5w)\left[1 + 0.5w + \frac{(0.5w)^2}{2}\right].$$

Hence,

$$P(W > 6) = 1 - F_W(6) = \exp(-0.5(6))\left[1 + 0.5(6) + \frac{(0.5 \times 6)^2}{2}\right] = 0.4232.$$

(d) This question involves the beta distribution. Let Z denote the time until the second bus arrives and let T denote the time between the second and third bus arriving. Then we want

$$P(Z + T > 2Z).$$

Rearranging $Z + T > 2Z$, we have that this is equivalent to

$$\frac{1}{2} > \frac{Z}{Z+T},$$

where

$$\frac{Z}{Z+T} = U \sim \text{Beta}(2, 1)$$

with U having p.d.f.

$$f_U(u) = \frac{(2+1-1)!}{(2-1)!(1-1)!} u^{2-1}(1-u)^{1-1} = 2u \qquad (0 < u < 1).$$

Hence

$$\begin{aligned} P(Z + T > 2Z) &= P(U < 0.5) \\ &= \int_0^{0.5} 2u\, du \\ &= \left[u^2\right]_0^{0.5} = 0.25. \end{aligned}$$

5.7 Normal (Gaussian) Distribution

Definition 5.7.1. **Normal (Gaussian) distribution.**

X is said to have a normal distribution, $X \sim N(\mu, \sigma^2)$, if it has p.d.f.

$$f_X(x) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left(-\frac{1}{2\sigma^2}[x-\mu]^2\right), \qquad x \in \mathbb{R},$$

where $\mu \in \mathbb{R}$ and $\sigma > 0$.

The parameters μ and σ of the normal distribution specify the mean and standard deviation with

$$E[X] = \int_{-\infty}^{\infty} x f_X(x)\, dx = \mu$$

and

$$E[X^2] = \int_{-\infty}^{\infty} x^2 f_X(x)\, dx = \sigma^2 + \mu^2$$

giving

$$var(X) = E[X^2] - E[X]^2 = \sigma^2.$$

The normal distribution is symmetric about its mean μ with the p.d.f. decreasing as $[x-\mu]^2$ increases. Therefore the median and mode of the normal distribution are also equal to μ. See Figure 5.6 for the p.d.f. and c.d.f. of $N(0,1)$.

Definition 5.7.2.
The c.d.f. of the normal distribution $X \sim N(\mu, \sigma^2)$ is

$$F_X(x) = \int_{-\infty}^{x} f(y)\, dy = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}[y-\mu]^2\right) dy,$$

and has no analytical solution. (*i.e.* We cannot solve the integral.)

How do we proceed with the Normal distribution if we cannot compute its c.d.f.?

The simplest solution is to use a statistical package such as **R** to compute probabilities (c.d.f.) for the Normal distribution. This can be done using the `pnorm` function. However, it is helpful to gain an understanding of the Normal distribution and how to compute probabilities (c.d.f.) for the Normal distribution using the good old-fashioned method of Normal distribution tables.

The starting point is to define the *standard normal distribution*, $Z \sim N(0,1)$. We can then show that for any $X \sim N(\mu, \sigma^2)$ and $a, b \in \mathbb{R}$, $P(a < X < b)$ can be rewritten as

$$P(a < X < b) = P(c < Z < d) = P(Z < d) - P(Z < c)$$

where c and d are functions of (a, μ, σ) and (b, μ, σ), respectively. It is thus sufficient to know the c.d.f. of Z. Note that when Z is used to define a normal distribution it will always be reserved for the standard normal distribution.

Traditionally, probabilities for Z are obtained from *Normal tables*, tabulated values of $P(Z < z)$ for various values of z. Typically, $P(Z < z)$ for $z = 0.00, 0.01, \ldots, 3.99$ are reported with the observation

$$P(Z < -z) = 1 - P(Z < z)$$

used to obtain probabilities for negative values.

A normal table will usually look similar to the table below.

z	0	1	2	3	4	⋯
0.0	0.5	0.504	0.508	0.512	0.516	⋯
0.1	0.5398	0.5438	0.5478	0.5517	0.5557	⋯
⋮	⋮	⋮	⋮	⋮	⋮	⋱
1.2	0.8849	0.8869	0.8888	0.8907	0.8925	⋯
⋮	⋮	⋮	⋮	⋮	⋮	⋱

The first column, labelled z, increments in units of 0.1. Columns 2 to 11 are headed 0 through to 9. To find $P(Z < z) = P(Z < r.st)$ where $z = r.st$ and r, s, t are integers between 0 and 9, inclusive, we look down the z column to the row $r.s$ and then look along the row to the column headed t. The entry in row "$r.s$" and column "t" is $P(Z < r.st)$. For example, $P(Z < 1.22) = 0.8888$.

Definition 5.7.3. **Standard Normal distribution.**

If $\mu = 0$ and $\sigma = 1$ then $Z \sim N(0,1)$ has a *standard normal* distribution with p.d.f.

$$\phi(x) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-x^2/2}, \quad x \in \mathbb{R},$$

and c.d.f.

$$\Phi(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-y^2/2} \, dy$$

Note the notation $\phi(\cdot)$ and $\Phi(\cdot)$ which are commonly used for the p.d.f. and c.d.f. of Z.

Lemma 5.7.4. **Transformation of a Normal random variable.**

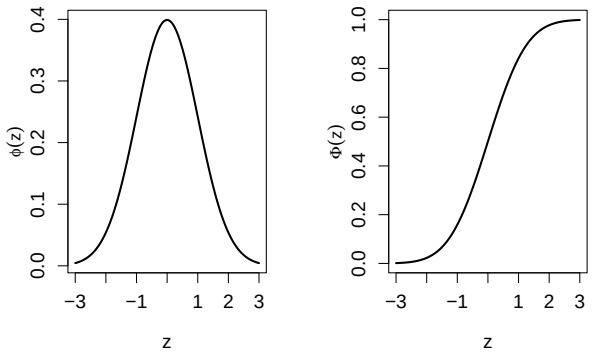


Figure 5.6: Standard normal, Z N(0,1), p.d.f. and c.d.f.

If $X \sim N(\mu, \sigma^2)$ and $Y = aX + b$ then

$$Y \sim N(a\mu + b, a^2\sigma^2).$$

An immediate Corollary of Lemma 5.7.4 is that if $X \sim N(\mu, \sigma^2)$, then

$$\frac{X - \mu}{\sigma} = Z \sim N(0, 1).$$

This corresponds to setting $a = 1/\sigma$ and $b = -\mu/\sigma$ in Lemma 5.7.4.

Hence, for any $x \in \mathbb{R}$,

$$P(X \leq x) = P\left(\frac{X - \mu}{\sigma} \leq \frac{x - \mu}{\sigma}\right) = P\left(Z \leq \frac{x - \mu}{\sigma}\right) = \Phi\left(\frac{x - \mu}{\sigma}\right).$$

Definition 5.7.5. **Percentage points**

The inverse problem of finding for a given q $(0 < q < 1)$, the value of z such that $P(Z < z) = q$ is often tabulated for important choices of q. The function `qnorm` in **R** performs this function for general $X \sim N(\mu, \sigma^2)$.

Definition 5.7.6. **Sums of Normal random variables**

Suppose that $X_1, X_2, \ldots, X_n$ are *independent* normal random variables with $X_i \sim N(\mu_i, \sigma_i^2)$. Then for $a_1, a_2, \ldots, a_n \in \mathbb{R}$,

$$Y = \sum_{i=1}^{n} a_i X_i \sim N\left(\sum_{i=1}^{n} a_i \mu_i, \sum_{i=1}^{n} a_i^2 \sigma_i^2\right).$$

Example 5.7.7. **Lemonade dispenser**

Suppose that the amount of lemonade dispensed by a machine into a cup is normally distributed with mean $250\,ml$ and standard deviation $5\,ml$. Suppose that the cups used for the lemonade are normally distributed with mean $260\,ml$ and standard deviation $4\,ml$.

(a) What is the probability that the lemonade overflows the cup?

(b) What is the probability that the total lemonade in 8 cups exceeds $1970ml$?

Attempt Example 5.7.7 (Lemonade dispenser) and then watch Video 13 for the solutions.

Watch Video 13: Lemonade dispenser

Solution to Example 5.7.7

(a) Let L and C denote the amount of lemonade dispensed and the size of a cup (in ml), respectively. Then $L \sim N(250, 5^2)$ and $C \sim N(260, 4^2)$, and we want:

$$P(C < L) = P(C - L < 0).$$

Note that $C - L$ follows a normal distribution (use Definition 5.7.6. Sums of Normal random variables with $n = 2$, $X_1 = C$, $X_2 = L$, $a_1 = 1$ and $a_2 = -1$) with $C - L \sim N(260 - 250, 25 + 16) = N(10, 41)$.

Therefore, if $Y \sim N(10, 41)$,

$$P(C < L) = P(Y < 0) = P\left(\frac{Y - 10}{\sqrt{41}} < \frac{0 - 10}{\sqrt{41}}\right) = \Phi\left(-1.56\right) = 0.0594.$$

Note that the answer is given by `pnorm(-1.56)` and for the answer rounded to 4 decimal places `round(pnorm(-1.56),4)`.

(b) Let $L_i \sim N(250, 5^2)$ denote the total number of lemonade dispensed into the i^{th} cup. Then the total amount of lemonade dispensed into 8 cups is $S = L_1 + L_2 + ... + L_8 \sim N(2000, 200)$. Therefore

$$P(S > 1970) = P\left(\frac{S - 2000}{\sqrt{200}} > \frac{1970 - 2000}{\sqrt{200}}\right) = P(Z > -2.12) = 1 - \Phi(-2.12) = 0.9830.$$

Student Exercises

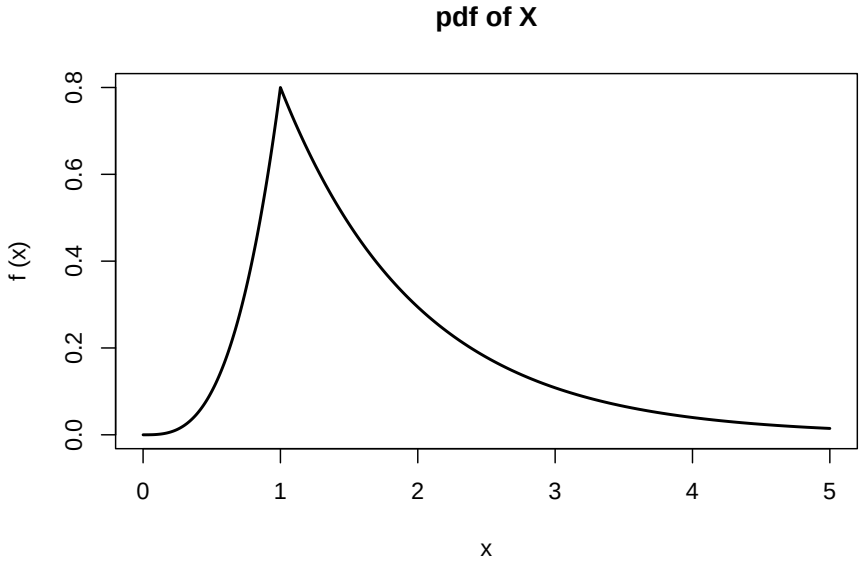
Attempt the exercises below.

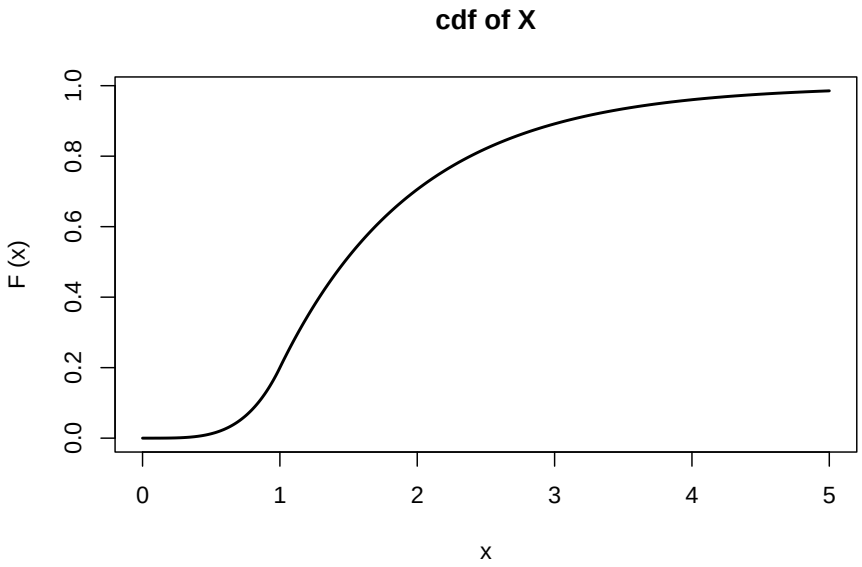
Exercise 5.1.
Let X be a continuous random variable with pdf

$$f_X(x) = \begin{cases} kx^3 & \text{if } 0 < x < 1, \\ ke^{1-x} & \text{if } x \geq 1, \\ 0 & \text{otherwise.} \end{cases}$$

(a) Evaluate k and find the (cumulative) distribution function of X.

(b) Calculate $P(0.5 < X < 2)$ and $P(X > 2|X > 1)$.





Exercise 5.2.
The time that a butterfly lives after emerging from its chrysalis is a random variable T, and the probability that it survives for more than t days is equal to $36/(6+t)^2$ for all $t > 0$.

(a) What is the probability that it will die within six days of emerging?

(b) What is the probability that it will live for between seven and fourteen days?

(c) If it has lived for seven days, what is the probability that it will live at least seven more days?

(d) If a large number of butterflies emerge on the same day, after how many days would you expect only 5% to be alive?

(e) Find the pdf of T.

(f) Calculate the mean life of a butterfly after emerging from its chrysalis.

Exercise 5.3.
A type of chocolate bar contains, with probability 0.1, a prize voucher. Whether or not a bar contains a voucher is independent of other bars. A hungry student buys 8 chocolate bars. Let X denote the number of vouchers that she finds.

(a) What sort of distribution does X have?

(b) How likely is it that the student finds no vouchers?

(c) How likely is it that she finds at least two vouchers?

(d) What is the most likely number of vouchers that she finds?

A second student keeps buying chocolate bars until he finds a voucher. Let Y denote the number of bars he buys.

(e) What is the probability mass function of Y?

(f) How likely is it that the student buys more than 5 bars?

(g) What is $E[Y]$?
(h) If each bar costs 35p, what is the expected cost to the student?

A third student keeps buying chocolate bars until they find 4 vouchers. In doing so, they buys a total of W bars.

(i) What is the distribution of W?

(j) What is the probability that this student buys exactly 10 bars?

Exercise 5.4.
A factory produces nuts and bolts on two independent machines. The external diameter of the bolts is normally distributed with mean 0.5 cm and the internal diameter of the nuts is normally distributed with mean 0.52 cm. The two machines have the same variance which is determined by the rate of production. The nuts and bolts are produced at rate which corresponds to a standard deviation $\sigma = 0.01$ cm and a third machine fits each nut on to the corresponding bolt as they are produced, provided the diameter of the nut is strictly greater than that of the bolt, otherwise it rejects both.

(a) Find the probability that a typical pair of nut and bolt is rejected.

(b) If successive pairs of nut and bolt are produced independently, find the probability that in 20 pairs of nut and bolt at least 1 pair is rejected.

(c) The management wishes to reduce the probability that a typical pair of nut and bolt is rejected to 0.01. What is the largest value of σ to achieve this?

Chapter 6

Joint Distribution Functions

6.1 Overview

In Section 5 we have introduced the concept of a random variable and a variety of discrete and continuous random variables. However, often in statistics it is important to consider the joint behaviour of two (or more) random variables. For example:

(i) Height, Weight.

(ii) Degree class, graduate salary.

In this section we explore the joint distribution between two random variables X and Y.

6.2 Joint c.d.f. and p.d.f.

Definition 6.2.1. **Joint c.d.f.**

The *joint (cumulative) probability distribution function* (joint c.d.f.) of X and Y is defined by

$$\begin{aligned} F_{X,Y}(x,y) &= P(\{\omega : X(\omega) \leq x \text{ and } Y(\omega) \leq y\}) \\ &= P(X \leq x, Y \leq y), \end{aligned}$$

where $x, y \in \mathbb{R}$.

Definition 6.2.2. **Joint p.d.f.**

Two r.v.'s X and Y are said to be *jointly continuous*, if there exists a function $f_{X,Y}(x,y) \geq 0$ such that for every "nice" set $C \subseteq \mathbb{R}^2$,

$$P((X,Y) \in C) = \int \int_C f_{X,Y}(x,y)\, dx\, dy.$$

The function $f_{X,Y}$ is called the *joint probability density function* (joint p.d.f.) of X and Y.

If X and Y are jointly continuous, then

$$\begin{aligned} F_{X,Y}(x,y) &= P(X \leq x, Y \leq y) \\ &= \int_{-\infty}^{y} \int_{-\infty}^{x} f_{X,Y}(u,v)\, du\, dv. \end{aligned}$$

Hence we differentiate the c.d.f. $F_{X,Y}(x,y)$ with respect to both x and y to obtain the p.d.f.

$$f_{X,Y}(x,y) = \frac{\partial^2}{\partial x \partial y} F_{X,Y}(x,y).$$

We note, as in the following example, that often the joint p.d.f. is non-zero on a subset of $\mathbb{R}^2$.

Example 6.2.3.
Suppose that

$$f_{X,Y}(x,y) = \begin{cases} 24x(1-x-y) & \text{if } x,y \geq 0 \text{ and } x+y \leq 1, \\ 0 & \text{otherwise.} \end{cases}$$

(a) Find $P(X > Y)$,

(b) Find $P(X > \frac{1}{2})$.

(a) Let $C = \{(x,y) : x > y\}$ and write $A = \{(x,y) : f_{X,Y}(x,y) > 0\}$. Then,

$$C \cap A = \{(x,y); x > 0, y > 0, x+y < 1, x > y\}.$$

Therefore

$$\begin{aligned}
P(X > Y) &= P((X,Y) \in C) \\
&= \int\int_C f_{X,Y}(x,y)\,dx\,dy \\
&= \int\int_{C\cap A} 24x(1-x-y)\,dx\,dy \\
&= \int_0^{1/2}\int_y^{1-y} 24x(1-x-y)\,dx\,dy \\
&= \int_0^{1/2} \left[12x^2 - 8x^3 - 12yx^2\right]_y^{1-y}\,dy \\
&= \int_0^{1/2} (4 - 12y + 16y^3)\,dy \\
&= \left[4y - 6y^2 + 4y^4\right]_0^{1/2} \\
&= 2 - \frac{3}{2} + \frac{1}{4} = \frac{3}{4}.
\end{aligned}$$

(b) Let $D = \{(x,y) : x > 1/2\}$, then

$$D \cap A = \{(x,y); x > 1/2, y > 0, x + y < 1\}.$$

Therefore

$$\begin{aligned}
P(X > 1/2) &= P((X,Y) \in D) \\
&= \int\int_D f_{X,Y}(x,y)\,dx\,dy \\
&= \int\int_{D\cap A} 24x(1-x-y)\,dx\,dy \\
&= \int_{1/2}^1 \int_0^{1-x} 24x(1-x-y)\,dy\,dx \\
&= \int_{1/2}^1 \left[24xy\left(1 - x - \frac{1}{2}y\right)\right]_0^{1-x} dx \\
&= \int_{1/2}^1 12x(1-x)^2\,dx \\
&= \left[\frac{12}{2}x^2 - \frac{24}{3}x^3 + \frac{12}{4}x^4\right]_{1/2}^1 \\
&= 6 - 8 + 3 - \frac{3}{2} + 1 - \frac{3}{16} = \frac{5}{16}.
\end{aligned}$$

6.3 Marginal c.d.f. and p.d.f.

There are many situations with bivariate distributions where we are interested in one of the random variables. For example, we might have the joint distribution of height and weight of individuals but only be interested in the weight of individuals. This is known as the **marginal distribution**.

Definition 6.3.1. **Marginal c.d.f.**

Suppose that the c.d.f. of X and Y is given by $F_{X,Y}$, then the c.d.f. of X can be obtained from $F_{X,Y}$ since

$$\begin{aligned} F_X(x) &= P(X \leq x) \\ &= P(X \leq x, Y < \infty) \\ &= \lim_{y \to \infty} F_{X,Y}(x, y). \end{aligned}$$

F_X is called the *marginal distribution* (marginal c.d.f.) of X.

Definition 6.3.2. **Marginal p.d.f.**

If $f_{X,Y}$ is the joint p.d.f. of X and Y, then the *marginal probability density function* (marginal p.d.f.) of X is given by

$$f_X(x) = \int_{-\infty}^{\infty} f_{X,Y}(x, y)\, dy.$$

Example 6.3.3
Consider Example 6.2.3.

Find the marginal p.d.f. and c.d.f of Y.

$$\begin{aligned} f_Y(y) &= \int_{-\infty}^{\infty} f_{X,Y}(x, y)\, dx \\ &= \begin{cases} \int_0^{1-y} 24x(1 - x - y)\, dx & 0 \leq y \leq 1, \\ 0 & \text{otherwise.} \end{cases} \\ &= \begin{cases} 4(1-y)^3 & 0 \leq y \leq 1, \\ 0 & \text{otherwise.} \end{cases} \end{aligned}$$

Note that marginal distribution of Y is a Beta$(1, 4)$ distribution.

Hence,

$$F_Y(y) = \begin{cases} 0, & y < 0, \\ \int_0^y 4(1-u)^3 du = 1-(1-y)^4, & 0 \le y \le 1, \\ 1, & y > 1. \end{cases}$$

Example 6.3.4.
Find the p.d.f. of $Z = X/Y$, where

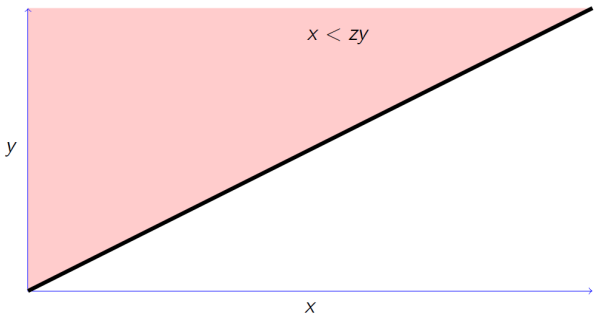
$$f_{X,Y}(x,y) = \begin{cases} e^{-(x+y)} & 0 < x, y < \infty, \\ 0 & \text{otherwise.} \end{cases}$$

Attempt Example 6.3.4 and then watch Video 14 for the solutions.

Watch Video 14: Ratio of Exponentials

Solution to Example 6.3.4.

Clearly, $Z > 0$. For $z > 0$,



Therefore

$$\begin{aligned} F_Z(z) &= P(Z \leq z) = P(X/Y \leq z) \\ &= \int\int_{\{(x,y):x/y\leq z\}} f_{X,Y}(x,y)\,dx\,dy \\ &= \int_0^\infty \int_0^{yz} e^{-(x+y)}\,dx\,dy \\ &= \int_0^\infty -e^{-y(1+z)} + e^{-y}\,dy \\ &= 1 - \frac{1}{1+z} \end{aligned}$$

and so

$$f_Z(z) = \frac{dF_Z(z)}{dz} = \begin{cases} \frac{1}{(1+z)^2}, & z > 0, \\ 0, & z \leq 0. \end{cases}$$

Note that we can extend the notion of joint and marginal distributions to random variables $X_1, X_2, \ldots, X_n$ in a similar fashion.

6.4 Independent random variables

Definition 6.4.1. **Independent random variables**

Random variables X and Y are said to be *independent* if, for all $x, y \in \mathbb{R}$,

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

that is, for all $x, y \in \mathbb{R}$, $F_{X,Y}(x,y) = F_X(x)F_Y(y)$.

If X and Y are discrete random variables with joint p.m.f. $p_{X,Y}(x,y)$ and marginal p.m.f.'s $p_X(x)$ and $p_Y(y)$, respectively, then X and Y are independent if and only if for all $x, y \in \mathbb{R}$,

$$p_{X,Y}(x,y) = p_X(x)p_Y(y).$$

If X and Y are continuous random variables with joint p.d.f. $f_{X,Y}(x,y)$ and marginal p.d.f.'s $f_X(x)$ and $f_Y(y)$, respectively, then X and Y are independent if and only if for all $x, y \in \mathbb{R}$,

$$f_{X,Y}(x,y) = f_X(x)f_Y(y).$$

For example, in Example 6.3.4 X and Y have joint probability density function:

$$\begin{aligned} f_{X,Y}(x,y) &= \exp(-\{x+y\}) \\ &= \exp(-x)\exp(-y) = f_X(x)f_Y(y), \quad (x,y>0), \end{aligned}$$

where both X and Y are distributed according to Exp(1). Thus the distribution Z given in Example 6.3.4 is the ratio of two independent exponential random variables with mean 1.

Note that we can easily extend the notion of independent random variables to random variables $X_1, X_2, \ldots, X_n$.

Definition 6.4.2. **Independent and identically distributed**

The random variables $X_1, X_2, \ldots, X_n$ are said to *independent and identically distributed* (i.i.d.) if,

- $X_1, X_2, \ldots, X_n$ are independent.
- $X_1, X_2, \ldots, X_n$ all have the same distribution, that is, $X_i \sim F$ for all $i = 1, \ldots, n$.

Definition 6.4.2 extends the notion of *i.i.d.* given at the start of Section 5.4.2 for discrete random variables.

Definition 6.4.3. **Random sample**

The random variables $X_1, X_2, \ldots, X_n$ are said to be a *random sample* if they are i.i.d.

Definition 6.4.4.
Suppose $X_1, X_2, \ldots, X_n$ are a random sample from the Poisson distribution with mean λ. Find the joint p.m.f. of $X_1, X_2, \ldots, X_n$.

If $X_i \sim \text{Po}(\lambda)$, then its p.m.f. is given by

$$P(X_i = x_i) = p_{X_i}(x_i) = \begin{cases} \frac{e^{-\lambda}\lambda^{x_i}}{x_i!} & \text{if } x_i = 0, 1, 2, \ldots, \\ 0 & \text{otherwise.} \end{cases}$$

Since $X_1, X_2, \ldots, X_n$ are independent, their joint p.m.f. is given by,

$$
\begin{aligned}
p_{X_1,X_2,\ldots,X_n}(x_1,x_2,\ldots,x_n) &= \prod_{i=1}^{n} p_{X_i}(x_i) \\
&= \begin{cases} \prod_{i=1}^{n} \frac{e^{-\lambda}\lambda^{x_i}}{x_i!} & \text{if } x_i = 0,1,2,\ldots, \\ 0 & \text{otherwise.} \end{cases} \\
&= \begin{cases} \frac{e^{-n\lambda}\lambda^{\sum_{i=1}^{n} x_i}}{\prod_{i=1}^{n} x_i!} & \text{if } x_i = 0,1,2,\ldots, \\ 0 & \text{otherwise.} \end{cases}
\end{aligned}
$$

The joint p.m.f. of $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ tells us how likely we are to observe $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ given λ. This can be used either:

1. To compute $P(\mathbf{X} = \mathbf{x})$ when λ is known;

2. Or, more commonly in statistics, to assess what is a *good estimate* of λ given $\mathbf{x}$ in situations where λ is unknown, see Parameter Estimation in Section 9.

Student Exercise

Attempt the exercise below.

Exercise 6.1.
A theory of chemical reactions suggests that the variation in the quantities X and Y of two products C_1 and C_2 of a certain reaction is described by the joint probability density function

$$f_{X,Y}(x,y) = \frac{2}{(1+x+y)^3} \qquad x \geq 0,\ y \geq 0.$$

On the basis of this theory, answer the following questions.

(a) What is the probability that at least one unit of each product is produced?

(b) Determine the probability that the quantity of C_1 produced is less than half that of C_2.

(c) Find the c.d.f. for the total quantity of C_1 and C_2.

Chapter 7

Central Limit Theorem and law of large numbers

7.1 Introduction

In this Section we will show why the Normal distribution, introduced in Section 5.7, is so important in probability and statistics. The central limit theorem states that under very weak conditions (almost all probability distributions you will see will satisfy them) the sum of n *i.i.d.* random variables, S_n, will converge, appropriately *normalised* to a standard Normal distribution as $n \to \infty$. For finite, but large $n(\geq 50)$, we can approximate S_n by a normal distribution and the normal distribution approximation can be used to answer questions concerning S_n. In Section 7.2 we present the **Central Limit Theorem** and apply it to an example using exponential random variables. In Section 7.3 we explore how a continuous distribution (the Normal distribution) can be used to approximate sums of discrete distributions. Finally, in Section 7.4, we present the **Law of Large Numbers** which states that the uncertainty in the sample mean of n observations, S_n/n, decreases as n increases and converges to the population mean μ. Both the Central Limit Theorem and the Law of Large Numbers will be important moving forward when considering statistical questions.

7.2 Statement of Central Limit Theorem

Before stating the **Central Limit Theorem**, we introduce some notation.

Definition 7.2.1. **Convergence in distribution**

A sequence of random variables $Y_1, Y_2, ...$ are said to **converge in distribution** to a random variable Y, if for all $y \in \mathbb{R}$,

$$P(Y_n \leq y) \to P(Y \leq y) \qquad \text{as } n \to \infty.$$

We write $Y_n \xrightarrow{D} Y$ as $n \to \infty$.

Theorem 7.2.2. **Central Limit Theorem.**
Let $X_1, X_2, \ldots, X_n$ be independent and identically distributed random variables (i.e. a random sample) with finite mean μ and variance σ^2. Let $S_n = X_1 + \cdots + X_n$. Then

$$\frac{S_n - n\mu}{\sigma\sqrt{n}} \xrightarrow{D} N(0,1).$$

The central limit theorem is equivalent to

$$\frac{\bar{X} - \mu}{\sigma/\sqrt{n}} \xrightarrow{D} N(0,1).$$

where $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$ is the mean of the distributions $X_1, X_2, \ldots, X_n$.

Therefore, we have that for large n,

$$S_n \approx N(n\mu, n\sigma^2)$$

and

$$\bar{X} \approx N\left(\mu, \frac{\sigma^2}{n}\right).$$

Example 7.2.3. Suppose $X_1, X_2, \ldots, X_{100}$ are i.i.d. exponential random variables with parameter $\lambda = 4$.

(a) Find $P(S_{100} > 30)$.

(b) Find limits within which $\bar{X}$ will lie with probability 0.95.

(a) Since $X_1, X_2, \ldots, X_{100}$ are i.i.d. exponential random variables with parameter $\lambda = 4$, $E[X_i] = \frac{1}{4}$ and $var(X_i) = \frac{1}{16}$. Hence,

$$E[S_{100}] = 100 \cdot \frac{1}{4} = 25;$$
$$var(S_{100}) = 100 \cdot \frac{1}{16} = \frac{25}{4}.$$

Since $n = 100$ is sufficiently big, S_{100} is approximately normally distributed by the central limit theorem (CLT). Therefore,

$$\begin{aligned} P(S_{100} > 30) &= P\left(\frac{S_{100} - 25}{\sqrt{\frac{25}{4}}} > \frac{30 - 25}{\sqrt{\frac{25}{4}}}\right) \\ &\approx P(N(0,1) > 2) \\ &= 1 - P(N(0,1) \leq 2) \\ &= 0.0228. \end{aligned}$$

Given that $S_{100} = \sum_{i=1}^{100} X_i \sim \text{Gamma}(100, 4)$, see Section 5.6.2, we can compute exactly $P(S_{100} > 30) = 0.0279$, which shows that the central limit theorem gives a reasonable approximation.

(b) Since $X_1, X_2, \ldots, X_{100}$ are i.i.d. exponential random variables with parameter $\lambda = 4$, $E[X_i] = \frac{1}{4}$ and $var(X_i) = \frac{1}{16}$. Therefore, $E\left[\bar{X}\right] = \frac{1}{4}$ and $var(\bar{X}) = \frac{1/16}{100}$.

Since $n = 100$, $\bar{X}$ will be approximately normally distributed by the CLT, hence

$$\begin{aligned} 0.95 &= P(a < \bar{X} < b) \\ &= P\left(\frac{a - 1/4}{\sqrt{1/1600}} < \frac{\bar{X} - 1/4}{\sqrt{1/1600}} < \frac{b - 1/4}{\sqrt{1/1600}}\right) \\ &\approx P\left(\frac{a - 1/4}{\sqrt{1/1600}} < N(0,1) < \frac{b - 1/4}{\sqrt{1/1600}}\right). \end{aligned}$$

There are infinitely many choices for a and b but a natural choice is $P(\bar{X} < a) = P(\bar{X} > b) = 0.025$. That is, we choose a and b such that there is equal chance that $\bar{X}$ is less than a or greater than b. Thus if for $0 < q < 1$, z_q satisfies $P(Z < z_q) = q$, we have that

$$\begin{aligned} \frac{a - 1/4}{\sqrt{1/1600}} &= z_{0.025} = -1.96, \\ \frac{b - 1/4}{\sqrt{1/1600}} &= z_{0.975} = 1.96. \end{aligned}$$

Hence,

$$a = 0.25 - 1.96\frac{1}{40} = 0.201,$$
$$b = 0.25 + 1.96\frac{1}{40} = 0.299.$$

7.3 Central limit theorem for discrete random variables

The central limit theorem can be applied to sums of discrete random variables as well as continuous random variables. Let $X_1, X_2, ...$ be *i.i.d.* copies of a discrete random variable X with $E[X] = \mu$ and $var(X) = \sigma^2$. Further suppose that the support of X is in the non-negative integers $\{0, 1, ...\}$. (This covers all the discrete distributions, we have seen, binomial, negative binomial, Poisson and discrete uniform.)

Let $Y_n \sim N(n\mu, n\sigma^2)$. Then the central limit theorem states that for large n, $S_n \approx Y_n$. However, there will exist $x \in \{0, 1, ...\}$ such that

$$P(S_n = x) > 0 \qquad \text{but} \qquad P(Y_n = x) = 0.$$

The solution is that we approximate

$$P(S_n = x) \qquad \text{by} \qquad P(x - 0.5 < Y_n \leq x + 0.5) = 0.$$

This is known as the **continuity correction**.

Example 7.3.1. Suppose that X is a Bernoulli random variable with $P(X = 1) = 0.6 (= p)$, so $E[X] = 0.6$ and $var(X) = 0.6 \times (1 - 0.6) = 0.24$. Then

$$S_n = \sum_{i=1}^{n} X_i \sim \text{Bin}(n, 0.6).$$

For $n = 100$, $S_{100} \sim \text{Bin}(100, 0.6)$ can be approximated by $Y \sim N(60, 24) (= N(np, np(1-p)))$, see Figure 7.1.

We can see the approximation in Figure 7.1 in close-up for $x = 54$ to 56 in Figure 7.2. The areas marked out by the red lines (normal approximation) are approximately equal to the areas of the bars in the histogram (binomial probabilities).

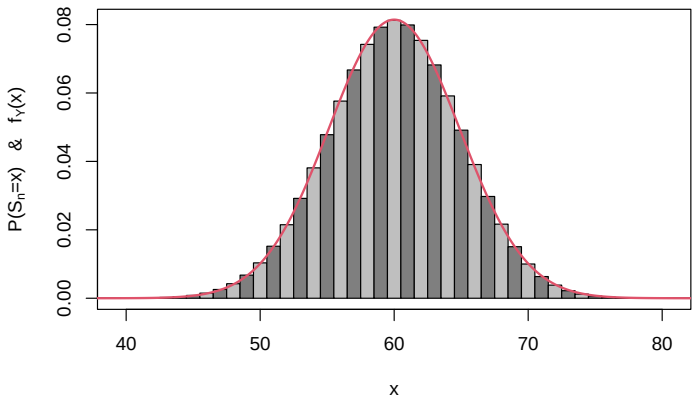


Figure 7.1: Central limit theorem approximation for the binomial.

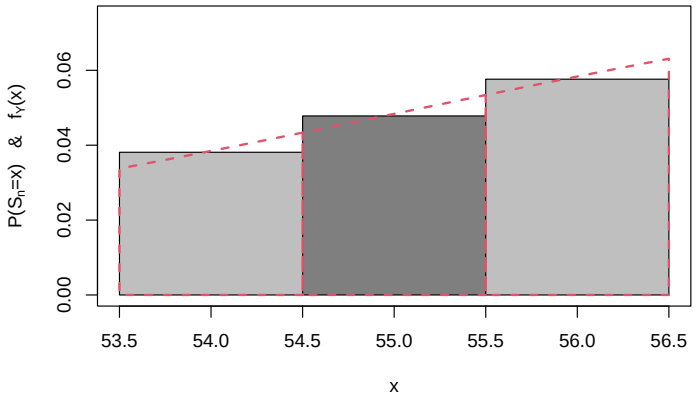


Figure 7.2: Central limit theorem approximation for the binomial for x=54 to 56.

7.4 Law of Large Numbers

We observed that

$$\bar{X} \approx N\left(\mu, \frac{\sigma^2}{n}\right),$$

and the variance is decreasing as n increases.

Given that

$$var(S_n) = var\left(\sum_{i=1}^{n} X_i\right) = \sum_{i=1}^{n} var\left(X_i\right) = n\sigma^2,$$

we have in general that

$$var(\bar{X}) = var\left(\frac{S_n}{n}\right) = \frac{1}{n^2} var(S_n) = \frac{\sigma^2}{n}.$$

A random variable Y which has $E[Y] = \mu$ and $var(Y) = 0$ is the *constant*, $Y \equiv \mu$, that is, $P(Y = \mu) = 1$. This suggests that as $n \to \infty$, $\bar{X}$ converges in some sense to μ. We can make this convergence rigorous.

Definition 7.4.1. **Convergence in probability**

A sequence of random variables $Y_1, Y_2, ...$ are said to **converge in probability** to a random variable Y, if for any $\epsilon > 0$,

$$P(|Y_n - Y| > \epsilon) \to 0 \qquad \text{as} \quad n \to \infty.$$

We write $Y_n \xrightarrow{p} Y$ as $n \to \infty$.

We will often be interested in convergence in probability where Y is a constant.

A useful result for proving convergence in probability to a constant μ is Chebychev's inequality. Chebychev's inequality is a special case of the Markov inequality which is helpful in bounding probabilities in terms of expectations.

Theorem 7.4.2. **Chebychev's inequality.**
Let X be a random variable with $E[X] = \mu$ and $var(X) = \sigma^2$. Then for any $\epsilon > 0$,

$$P(|X - \mu| > \epsilon) \leq \frac{\sigma^2}{\epsilon^2}.$$

Theorem 7.4.3. **Law of Large Numbers.**
Let $X_1, X_2, ...$ be *i.i.d.* according to a random variable X with $E[X] = \mu$ and $var(X) = \sigma^2$. Then

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i \xrightarrow{p} \mu \qquad \text{as} \quad n \to \infty.$$

First, note that

$$E[\bar{X}] = E\left[\frac{1}{n}\sum_{i=1}^{n} X_i\right] = \frac{1}{n}\sum_{i=1}^{n} E\left[X_i\right] = \frac{1}{n}(n\mu) = \mu.$$

For any $\epsilon > 0$, we have by Chebychev's inequality that

$$P(|\bar{X} - \mu| > \epsilon) \leq \frac{1}{\epsilon^2} var(\bar{X}) = \frac{\sigma^2}{n\epsilon^2} \to 0 \qquad \text{as } n \to \infty,$$

and the Theorem follows.

Example 7.4.4. **Central limit theorem for dice**

Figure 7.3: Dice picture.

Let $D_1, D_2, ...$ denote the outcomes of successive rolls of a fair six-sided dice.

Let $S_n = \sum_{i=1}^{n} D_i$ denote the total score from n rolls of the dice and let $M_n = \frac{1}{n} S_n$ denote the mean score from n rolls of the dice.

(a) What is the approximate distribution of S_{100}?

(b) What is the approximate probability that S_{100} lies between 330 and 380, inclusive?

(c) How large does n need to be such that $P(|M_n - E[D]| > 0.1) \leq 0.01$?

Attempt Example 7.4.4 and then watch Video 15 for the solutions.

Watch Video 15: Central limit theorem for dice

Solution to Example 7.4.4.

Note that D_1 is a discrete uniform distribution with probability mass function

$$P(D_1 = x) = \begin{cases} \frac{1}{6} & x = 1, 2, \ldots, 6, \\ 0 & \text{otherwise.} \end{cases}$$

Then $E[D_1] = \frac{7}{2} = 3.5$ and $Var(D_1) = \frac{35}{12}$.

(a) Since the rolls of the dice are independent,

$$\begin{aligned} E[S_{100}] &= E\left[\sum_{i=1}^{100} D_i\right] = \sum_{i=1}^{100} E\left[D_i\right] \\ &= 100E[D_1] = 350. \end{aligned}$$

and

$$\begin{aligned} var(S_{100}) &= var\left(\sum_{i=1}^{100} D_i\right) = \sum_{i=1}^{100} var\left(D_i\right) \\ &= 100var(D_1) = \frac{875}{3}. \end{aligned}$$

Thus by the central limit theorem, $S_{100} \approx Y \sim N\left(350, \frac{875}{3}\right)$.

(b) Using the CLT approximation above, and the continuity correction

$$\begin{aligned} P(330 \leq S_{100} \leq 380) &\approx P(329.5 \leq Y \leq 380.5) \\ &= P(Y \leq 380.5) - P(Y \leq 329.5) \\ &= 0.9629 - 0.115 = 0.8479. \end{aligned}$$

If using Normal tables, we have that

$$P\left(Y \leq 380.5\right) = P\left(Z = \frac{Y - 350}{\sqrt{875/3}} \leq \frac{380.5 - 350}{\sqrt{875/3}}\right) = \Phi(1.786)$$

and

$$P\left(Y \leq 329.5\right) = P\left(Z = \frac{Y - 350}{\sqrt{875/3}} \leq \frac{329.5 - 350}{\sqrt{875/3}}\right) = \Phi(-1.200).$$

(c) Using the Central Limit Theorem, $M_n \approx W_n \sim N\left(\frac{7}{2}, \frac{35}{12n}\right)$.

We know by the law of large numbers that $M_n \xrightarrow{p} \frac{7}{2}$ as $n \to \infty$, but how large does n need to be such that there is a 99% (or greater) chance of M_n being within 0.1 of 3.5?

Using the approximation W_n, we want:

$$P\left(\left|W_n - \frac{7}{2}\right| > 0.1\right) \leq 0.01.$$

Now equivalently we want n such that

$$\begin{aligned} 0.99 &\geq P(3.4 \leq W_n \leq 3.6) \\ &= P\left(\frac{3.4 - 3.5}{\sqrt{35/(12n)}} \leq Z \leq \frac{3.6 - 3.5}{\sqrt{35/(12n)}}\right) \\ &= P\left(-0.058554\sqrt{n} < Z < 0.58554\sqrt{n}\right) \\ &= P(|Z| < 0.058554\sqrt{n}) = 1 - P(|Z| > 0.058554\sqrt{n}). \end{aligned}$$

Consider $P(|Z| > 0.058554\sqrt{n}) = 0.01$.
Note that

$$P(|Z| > c) = \alpha \qquad \Leftrightarrow \qquad P(Z > c) = \frac{\alpha}{2} \qquad \Leftrightarrow \qquad P(Z \leq c) = 1 - \frac{\alpha}{2}.$$

We have $\alpha = 0.01$, and using `qnorm` function in **R** `qnorm(0.995)` gives $c = 2.5758293$.
Therefore

$$P(|Z| > 0.058554\sqrt{n}) = 0.01 = P(|Z| > 2.5758),$$

or equivalently

$$0.058554\sqrt{n} = 2.5758 \qquad \Rightarrow \qquad \sqrt{n} = 43.99 \qquad \Rightarrow \qquad n = 1935.2.$$

Given that we require $n \geq 1935.2$, we have that $n = 1936$.

Task: Session 4

Attempt the **R Markdown** file for Session 4:
Session 4: Convergence and the Central Limit Theorem

Student Exercises

Attempt the exercises below.

Exercise 7.1.
Let $X_1, X_2, \ldots, X_{25}$ be independent Poisson random variables each having mean 1. Use the central limit theorem to approximate

$$P\left(\sum_{i=1}^{25} X_i > 20\right).$$

Exercise 7.2.
The lifetime of a Brand X TV (in years) is an exponential random variable with mean 10. By using the central limit theorem, find the approximate probability that the average lifetime of a random sample of 36 TVs is at least 10.5.

Exercise 7.3.
Prior to October 2015, in the UK National Lottery gamblers bought a ticket on which they mark six different numbers from $\{1, 2, \ldots, 49\}$. Six balls were drawn uniformly at random without replacement from a set of 49 similarly numbered balls. A ticket won the jackpot if the six numbers marked are the same as the six numbers drawn.

(a) Show that the probability a given ticket won the jackpot is 1/13983816.

(b) In Week 9 of the UK National Lottery $69,846,979$ tickets were sold and there were 133 jackpot winners. If all gamblers chose their numbers independently and uniformly at random, use the central limit theorem to determine the approximate distribution of the number of jackpot winners that week. Comment on this in the light of the actual number of jackpot winners.

Chapter 8

Motivation for Statistical Inference

8.1 Introduction

In Section 1, we introduced the statistical paradigm and the concepts of a population and a sample (see Section 1.2). We have seen a range of statistics, in particular, those for measuring location (mean, median, mode) and those for measuring spread (variance, interquartile range, range) derived from a sample. In the proceeding sections we have introduced probability as a means for measuring and encapsulating uncertainty. We now begin to combine these ideas to link *sample* statistics to *population* statistics.

8.2 Motivating example

From a sample of 52 university students, four individuals were found to be left-handed. We can easily summarise the sample information as the proportion $\frac{4}{52} = \frac{1}{13}$. However:

- What are we able to say about the population?
- What proportion of all university students are left-handed?
- Is $\frac{1}{13}$ a good estimate and what do we mean by *'good"*?

We identify the important features of statistical inference in this example. Here, the *population* are all university students. The population has some *parameter* or characteritic, θ, which we wish to estimate. In this example, θ is the probability of an individual being left-handed.

From the population we take a *random sample* which means each member of the population has an equal chance of being chosen. The sample gives rise to *data* $x_1, x_2, \ldots, x_n$. We estimate the parameter θ by means of a *statistic* $T(x_1, x_2, \ldots, x_n)$.

8.3 Modelling assumptions

1. **Identically distributed assumption:** Every sample observation (data point) x is the outcome of a random variable X which has an identical distribution (either discrete or continuous) for every member of the population.
2. **Independence assumption:** The random variables $X_1, X_2, \ldots, X_n$ which give rise to the data points $x_1, x_2, \ldots, x_n$ are independent.

Note that we defined a random sample to be a set of i.i.d. random variables. See Section 6.4 for further details on independence and identically distributed.

The subtle point here is that we are treating the observed data as just one possible outcome from the many different outcomes that could occur.

8.4 Parametric models

In the parametric approach to statistics (inference), we assume that the random sample that we collect was generated by some specific probability distribution which is completely known, except for a small number of parameters. For example:

- we could assume that the annual income in the U.K. is normally distributed but we don't know its mean, μ, or its variance, σ^2;
- in studying the effectiveness of a certain drug's ability to decrease the size of tumours in laboratory rats, we assume that the outcome of the tumour size being decreased (or not) has a Binomial distribution where n is the known sample size and p is the unknown probability of a successful treatment of one tumour.

There are a number of approaches to determine the underlying model that should be used:

- Physical argument, *e.g.* counts of events from a Poisson process follow a Poisson distribution;
- Mathematical argument, *e.g.* central limit theorem leading to a normal distribution;
- Flexible model which fairly arbitrarily covers a wide range of possibilities.

Chapter 9

Parameter Estimation

9.1 Introduction

In this section, we consider the general definition of a statistic as a summary of a random sample. Statistics are used as *estimators* of population quantities with an *estimate* denoting a given realisation of an estimator. We explore key properties that we wish estimators to have such as *unbiasedness*, *efficiency* and *consistency*. We study the properties of the sample mean and sample variance as estimators of the population mean and variance, respectively.

9.2 Preliminaries

Definition 9.2.1. **Statistic**

A *statistic*, $T(\mathbf{X})$, is any function of the random sample.

Note that since $T(\mathbf{X})$ is a function of random variables, it is also a random variable. Hence it will also have all the properties of a random variable. Most importantly, it has a distribution associated with it.

Definition 9.2.2. **Estimator**

A statistic that is used for the purpose of estimating an unknown population parameter is called an *estimator*.

Definition 9.2.3. **Estimate**

A realised value of an estimator, $T(\mathbf{x})$, that is the value of $T(\mathbf{X})$ evaluated at a particular outcome of the random sample, is called an *estimate*.

That is, if we let $Y = T(\mathbf{X})$ then Y is a random variable and $y = T(\mathbf{x})$ is a realisation of the random variable Y based on the sample $\mathbf{x} = (x_1, x_2, \dots, x_n)$.

The properties of the estimator $T(\mathbf{X})$ will typically depend upon n, the number of observations in the random sample.

Example 9.2.4. **Average Income**

Suppose that we want to estimate the average annual income in the U.K. Let $X_1, X_2, \ldots, X_n$ be a random sample of annual incomes. Possible estimators might include:

- $T_1(\mathbf{X}) = \frac{X_1+X_2+\cdots+X_n}{n}$;
- $T_2(\mathbf{X}) = \min\{X_1, X_2, \ldots, X_n\}$;
- $T_3(\mathbf{X}) = X_1$.

Which of these is the best choice of estimator?

9.3 Judging estimators

Let θ be a population parameter we wish to estimate. Since any function of the sample data is a potential estimator of θ, how should we determine whether an estimator is good or not? What qualities should our estimator have?

Quality 1: Unbiasedness

Definition 9.3.1. **Unbiased**

The estimator $T(\mathbf{X})$ is an *unbiased* estimate of θ if

$$E\left[T(\mathbf{X})\right] = \theta.$$

Otherwise, we say that the estimator $T(\mathbf{X})$ is biased and we define

$$B(T) = E\left[T(\mathbf{X})\right] - \theta$$

to be the *bias* of T.

Asymptotically unbiased
Definition 9.3.2. If $B(T) \to 0$ as the sample size $n \to \infty$, then we say that $T(\mathbf{X})$ is *asymptotically unbiased* for θ.

Quality 2: Small variance

Definition 9.3.3. **Efficiency**

If two estimators $T_1(\mathbf{X})$ and $T_2(\mathbf{X})$ are both unbiased for θ, then $T_1(\mathbf{X})$ is said to be *more efficient* than $T_2(\mathbf{X})$ if

$$var\left(T_1(\mathbf{X})\right) < var\left(T_2(\mathbf{X})\right).$$

We would ideally like an estimator that is unbiased with a small variance. So given multiple unbiased estimators, we choose the most efficient estimator (the estimator with the smallest variance).

For comparing an estimator with a biased estimator, we can use the mean-square error to quantify the trade-off between bias and variance:

Definition 9.3.1. **Mean-square error**

The *mean-square error* of an estimator is defined by

$$\text{MSE}(T) = E\left[(T(\mathbf{X}) - \theta)^2\right].$$

Example 9.3.5. Prove $\text{MSE}(T) = \text{var}(T) + (B(T))^2$.

Watch Video 16 for the proof of Example 9.3.5.

Watch Video 16: Derivation of MSE

Proof of Example 9.3.5.

The first step is to note that we can write

$$\begin{aligned} T(\mathbf{X}) - \theta &= T(\mathbf{X}) - E[T(\mathbf{X})] + E[T(\mathbf{X})] - \theta \\ &= T(\mathbf{X}) - E[T(\mathbf{X})] + B(T). \end{aligned}$$

Therefore

$$\begin{aligned} E\left[(T(\mathbf{X}) - \theta)^2\right] &= E\left[(T(\mathbf{X}) - E[T(\mathbf{X})] + B(T))^2\right] \\ &= E\left[(T(\mathbf{X}) - E[T(\mathbf{X})])^2 + 2B(T)\left(T(\mathbf{X}) - E[T(\mathbf{X})]\right) + B(T)^2\right] \\ &= E\left[(T(\mathbf{X}) - E[T(\mathbf{X})])^2\right] + 2E\left[B(T)\left(T(\mathbf{X}) - E[T(\mathbf{X})]\right)\right] + E\left[B(T)^2\right]. \end{aligned}$$

Since $B(T)$ is a constant, the middle term in the above equation is

$$\begin{aligned} 2E\left[B(T)\left(T(\mathbf{X}) - E[T(\mathbf{X})]\right)\right] &= 2B(T)E\left[T(\mathbf{X}) - E[T(\mathbf{X})]\right] \\ &= 2B(T)\left\{E[T(\mathbf{X})] - E[T(\mathbf{X})]\right\} = 0. \end{aligned}$$

Therefore, since $E\left[(T(\mathbf{X}) - E[T(\mathbf{X})])^2\right] = var(T(\mathbf{X}))$, we have that

$$E\left[(T(\mathbf{X}) - \theta)^2\right] = var(T(\mathbf{X})) + 0 + B(T)^2$$

as required.

Quality 3: Consistency

Definition 9.3.6. **Consistency**

An estimator $T(\mathbf{X})$ is said to be a *consistent* estimator for θ if

$$T(\mathbf{X}) \xrightarrow{p} \theta, \qquad \text{as } n \to \infty.$$

Remember convergence in probability ($\xrightarrow{p}$) is defined in Section 7.4, and the definition of consistency implies that, for any $\epsilon > 0$,

$$P(|T(\mathbf{X}) - \theta| > \epsilon) \to 0 \qquad \text{as } n \to \infty.$$

That is, as n becomes large the probability that $T(\mathbf{X})$ differs from θ by more than ϵ, for any positive ϵ, becomes small and goes to 0 as $n \to \infty$.

This third desirable property can sometimes be established using the following theorem:

Theorem 9.3.7. **Consistency Theorem**

If $E[T(\mathbf{X})] \to \theta$ and $\text{Var}(T(\mathbf{X})) \to 0$ as $n \to \infty$, then $T(\mathbf{X})$ is a consistent estimator for θ.

Note that the **Consistency Theorem** gives sufficient but not necessary conditions for consistency. Since by Example 9.3.5 $\text{MSE}(T) = \text{var}(T) + (B(T))^2$, the **Consistency Theorem** implies that if $\text{MSE}(T) \to 0$ as $n \to \infty$, then $T(\mathbf{X})$ is a consistent estimator for θ.

Example 9.3.8.
Suppose $X_1, X_2, \ldots, X_n$ is a random sample from any population with mean μ and variance σ^2. The sample mean is $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$ and is an estimator of μ. What are the properties of $\bar{X}$?

Firstly, we can show that $\bar{X}$ is unbiased:

$$\begin{aligned} E[\bar{X}] &= E\left[\frac{1}{n}(X_1 + X_2 + \ldots + X_n)\right] \\ &= \frac{1}{n}\{E[X_1] + E[X_2] + \ldots + E[X_n]\} \\ &= \frac{1}{n}\{\mu + \mu + \ldots + \mu\} \\ &= \frac{1}{n} n\mu \\ &= \mu. \end{aligned}$$

The variance of $\bar{X}$ is $\frac{\sigma^2}{n}$ since:

$$\begin{aligned} var(\bar{X}) &= var\left(\frac{1}{n}\sum_{i=1}^{n} X_i\right) \\ &= \frac{1}{n^2}\sum_{i=1}^{n} \mathrm{Var}(X_i) \\ &= \frac{1}{n^2}\sum_{i=1}^{n} \sigma^2 \\ &= \frac{1}{n^2} n\sigma^2 \\ &= \frac{\sigma^2}{n}. \end{aligned}$$

Given that $\bar{X}$ is an unbiased estimator the mean-square error of $\bar{X}$ is equal to $var(\bar{X}) = \frac{\sigma^2}{n}$.

Since $E[\bar{X}] \to \mu$ and $var(\bar{X}) \to 0$ as $n \to \infty$, it follows from the **Consistency Theorem** that $\bar{X}$ is a consistent estimator for μ.

We return to Average Income Example concerning the average annual income in the UK.

It follows from Example 9.3.8 that

$$T_1(\mathbf{X}) = \frac{X_1 + X_2 + ... + X_n}{n}$$

is an unbiased and consistent estimator of the mean annual income.

Let L denote the lowest annual income in the UK. Then

$$T_2(\mathbf{X}) = \min\{X_1, X_2, ..., X_n\} \to L \qquad \text{as } n \to \infty.$$

Except in the case $n = 1$, the mean of $T_2(\mathbf{X})$ will be below the mean annual income (the exact value will depend on the distribution of annual incomes) and will become smaller as n increases with the limit L as $n \to \infty$.

The final estimator $T_3(\mathbf{X}) = X_1$ is unbiased as $E[X_1]$ is the average annual income. However, for all $n = 1, 2, ...$, $var(T_3(\mathbf{X})) = var(X_1)$ and unless the annual income is constant, $var(X_1) > 0$. Therefore $T_3(\mathbf{X})$ is not a consistent

estimator since the estimator, and hence its variance, does not change as we increase the sample size.

9.4 Sample Variance

Example 9.4.1. **Variance Estimator**

Suppose $X_1, X_2, \ldots, X_n$ is a random sample from any population with mean μ and variance σ^2. Consider the estimator

$$\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}\left(X_i - \bar{X}\right)^2.$$

Before considering the estimator $\hat{\sigma}^2$ in Example 9.4.1 we prove Lemma 9.4.2 which is useful in manipulating sums of squares.

Lemma 9.4.2. **Splitting square**

$$\begin{aligned}\sum_{i=1}^{n}(X_i-\mu)^2 &= \sum_{i=1}^{n}(X_i-\bar{X})^2+\sum_{i=1}^{n}(\bar{X}-\mu)^2\\ &= \sum_{i=1}^{n}(X_i-\bar{X})^2+n(\bar{X}-\mu)^2.\end{aligned}$$

The proof uses the same approach to that given for the $MSE(T)$ in Example 9.3.5 in that we can write

$$\begin{aligned}\sum_{i=1}^{n}(X_i-\mu)^2 &= \sum_{i=1}^{n}(X_i-\bar{X}+\bar{X}-\mu)^2\\ &= \sum_{i=1}^{n}\left\{(X_i-\bar{X})^2+2(X_i-\bar{X})(\bar{X}-\mu)+(\bar{X}-\mu)^2\right\}\\ &= \sum_{i=1}^{n}(X_i-\bar{X})^2+2(\bar{X}-\mu)\sum_{i=1}^{n}(X_i-\bar{X})+\sum_{i=1}^{n}(\bar{X}-\mu)^2.\end{aligned}$$

Note that

$$\sum_{i=1}^{n}(X_i-\bar{X})=\sum_{i=1}^{n}X_i-n\bar{X}=n\bar{X}-n\bar{X}=0,$$

and the Lemma follows.

Lemma 9.4.2 is an example of a common trick in statistics. Suppose that we have $A_i = B_i + K$ $(i = 1, 2, \ldots, n)$ such that $\sum_{i=1}^{n} B_i = 0$, then

$$\sum_{i=1}^{n} A_i^2 = \sum_{i=1}^{n} (B_i + K)^2 = \sum_{i=1}^{n} B_i^2 + nK^2.$$

We check whether the variance estimator $\hat{\sigma}^2$ is biased or unbiased:

$$\begin{aligned}
E[\hat{\sigma}^2] &= E\left[\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2\right] \\
&= E\left[\frac{1}{n}\sum_{i=1}^{n}(X_i - \mu)^2 - \frac{1}{n}\sum_{i=1}^{n}(\bar{X} - \mu)^2\right] \\
&= \frac{1}{n}\sum_{i=1}^{n} E\left[(X_i - \mu)^2\right] - \frac{1}{n}\sum_{i=1}^{n} E\left[(\bar{X} - \mu)^2\right] \\
&= \frac{1}{n}\sum_{i=1}^{n} \mathrm{Var}(X_i) - \frac{1}{n}\sum_{i=1}^{n} \mathrm{Var}(\bar{X}) \\
&= \frac{1}{n} n\sigma^2 - \frac{1}{n} n \frac{\sigma^2}{n} \\
&= \frac{(n-1)\sigma^2}{n}.
\end{aligned}$$

Hence $E[\hat{\sigma}^2] \neq \sigma^2 = Var(X_i)$ and so $\hat{\sigma}^2$ is a **biased**, although asymptotically unbiased, estimator for σ^2. Under weak additional conditions, such as $E[X_1^4] < \infty$, it can be shown that $\hat{\sigma}^2$ is a consistent estimator.

It follows from Variance Estimator that given a random sample $X_1, X_2, \ldots, X_n$, the quantity,

$$s^2 = \frac{n}{n-1}\hat{\sigma}^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2$$

is an unbiased estimator of σ^2. This is the definition of the sample variance that we gave in Section 2.3.

It can be shown that

$$s^2 = \frac{1}{n-1}\left(\sum_{i=1}^{n} X_i^2 - \frac{\left(\sum_{i=1}^{n} X_i\right)^2}{n}\right) = \frac{1}{n-1}\left(\sum_{i=1}^{n} X_i^2 - n\bar{X}^2\right).$$

Definition 9.4.3. **Sample variance and covariance**

Given observed data $x_1, x_2, \ldots, x_n$, then we define the *sample variance* by

$$s_x^2 = \frac{1}{n-1}\sum_{i=1}^{n}(\bar{x}_i - \bar{x})^2 = \frac{1}{n-1}\left(\sum_{i=1}^{n} x_i^2 - \frac{\left(\sum_{i=1}^{n} x_i\right)^2}{n}\right) = \frac{1}{n-1}\left(\sum_{i=1}^{n} x_i^2 - n\bar{x}^2\right).$$

Similarly, if we have data pairs $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ we define the *sample covariance* by:

$$s_{xy} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}).$$

Task: Session 5

Attempt the **R Markdown** file for Session 5:
Session 5: Estimators

Student Exercises

Attempt the exercises below.

Exercise 9.1.
Suggest a reasonable statistical model for each of the following situations, and say which parameter or function of the parameter(s) in the model is likely to be of main interest:

(a) The number of reportable accidents that occur in the University in the month of October is ascertained, with a view to estimating the overall accident rate for the academic year;

(b) In a laboratory test the times to failure of 10 computer hard disk units are measured, to enable the manufacturer to quote for the *mean time to failure* in sales literature.

Of course in practice one needs to check whether the suggested models are reasonable, e.g. by examining a histogram.

Exercise 9.2.
Suppose that a surveyor is trying to determine the area of a rectangular field, in which the measured length Y_1 and the measured width Y_2 are independent random variables taking values according to the following distributions:

y_1	8	10	11
$p(y_1)$	0.25	0.25	0.5

y_2	4	6
$p(y_2)$	0.5	0.5

The calculated area $A = Y_1Y_2$ is also a random variable, and is used to estimate the true area. If the true length and width are 10 and 5, respectively.

(a) Is Y_1 an unbiased estimator of the true length?

(b) Is Y_2 an unbiased estimator of the true width?

(c) Is A an unbiased estimator of the true area?

Chapter 10

Techniques for Deriving Estimators

10.1 Introduction

In this Section we introduce two techniques for deriving estimators:

- Method of Moments
- Maximum Likelihood Estimation

The Method of Moments is a simple, intuitive approach, which has its limitations beyond simple random sampling (*i.i.d.* observations). Maximum Likelihood Estimation is an approach which can be extended to complex modelling scenarios and likelihood based estimation will be central to statistical inference procedures throughout not only this module but the whole course.

10.2 Method of Moments

Let X be a random variable.

Definition 10.2.1. **Moments**

If $E[X^k]$ exists in the sense that it is finite, then $E[X^k]$ is said to be the k^{th} *moment* of the random variable X.

For example,

- $E[X] = \mu$ is the first moment of X;
- $E[X^2]$ is the second moment of X.

Note that $var(X) = E[X^2] - (E[X])^2$ is a function of the first and second moments.

Definition 10.2.2. **Sample moments**

Let $X_1, X_2, \ldots, X_n$ be a random sample. The k^{th} *sample moment* is

$$\hat{\mu}_k = \frac{1}{n}\sum_{i=1}^{n} X_i^k.$$

Since,

$$\begin{aligned} E[\hat{\mu}_k] &= E\left[\frac{1}{n}\sum_{i=1}^{n} X_i^k\right] \\ &= \frac{1}{n}\sum_{i=1}^{n} E\left[X_i^k\right] \\ &= E\left[X_i^k\right], \end{aligned}$$

it follows that the k^{th} sample moment is an unbiased estimator of the k^{th} moment of a distribution. Therefore, if one wants to estimate the parameters from a particular distribution, one can write the parameters as a function of the moments of the distribution and then estimate them by their corresponding sample moments. This is known as the **method of moments**.

Lemma 10.2.3. **Method of Moments: Mean and Variance**

Let $X_1, X_2, \ldots, X_n$ be a random sample from any distribution with mean μ and variance σ^2.
The method of moments estimators for μ and σ^2 are:

$$\hat{\mu} = \bar{X} \qquad \text{and} \qquad \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2.$$

The method of moments estimator for μ is

$$\begin{aligned} \hat{\mu} &= \hat{\mu}_1 \\ &= \frac{1}{n}\sum_{i=1}^{n} X_i \\ &= \bar{X}, \end{aligned}$$

Given that $\sigma^2 = E[X^2] - E[X]^2$, the method of moments estimator for σ^2 is

$$\begin{aligned}\hat{\sigma}^2 &= \hat{\mu}_2 - (\hat{\mu}_1)^2 \\ &= \frac{1}{n}\sum_{i=1}^{n} X_i^2 - \left(\frac{1}{n}\sum_{i=1}^{n} X_i\right)^2 \\ &= \frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2.\end{aligned}$$

Note that $E[\hat{\mu}] = E[\bar{X}] = \mu$ is an unbiased estimator, whilst

$$E[\hat{\sigma}^2] = E\left[\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2\right] = \frac{n-1}{n}\sigma^2$$

is a biased estimator, but is asymptotically unbiased. See Section 9.4 where the properties of $\hat{\sigma}^2$ are explored further.

Example 10.2.4. **Method of Moments: Binomial distribution**

Let $X_1, X_2, \ldots, X_n \sim \text{Bin}(m, \theta)$ where m is known. Find the method of moments estimator for θ.

The first moment (mean) of the Binomial distribution is $m\theta$. Therefore,

$$\hat{\theta} = \frac{\hat{\mu}_1}{m} = \frac{\bar{X}}{m}.$$

Example 10.2.5. **Method of Moments: Exponential distribution**

Let $X_1, X_2, \ldots, X_n \sim \text{Exp}(\theta)$. Find the method of moments estimator for θ.

For $x > 0$ and $\theta > 0$,

$$f(x|\theta) = \theta e^{-\theta x}.$$

Therefore $E[X] = 1/\theta$, so $1/\hat{\theta} = \bar{X}$ and

$$\hat{\theta} = 1/\bar{X}.$$

The sampling properties of the k^{th} sample moment are fairly desirable:

- $\hat{\mu}_k$ is an unbiased estimator of $E[X^k]$;
- By the Central Limit Theorem, $\hat{\mu}_k$ is asymptotically normal if $E[X^{2k}]$ exists;
- $\hat{\mu}_k$ is a consistent estimator of $E[X^k]$.

If h is a continuous function, then $\hat{\theta} = h(\hat{\mu}_1, \hat{\mu}_2, \dots, \hat{\mu}_k)$ is a consistent estimator of $\theta = h(\mu_1, \mu_2, \dots, \mu_k)$, but it may not be an unbiased or an asymptotically normal estimator.

There are often difficulties with the method of moments:

- Finding θ as a function of theoretical moments is not always simple;
- For some models, moments may not exist.

10.3 Maximum likelihood estimation

In the study of probability, for random variables $X_1, X_2, \dots, X_n$ we consider the joint probability mass function or probability density function as just a function of the random variables $X_1, X_2, \dots, X_n$. Specifically we assume that the parameter value(s) are completely known.

For example, if $X_1, X_2, \dots, X_n$ is a random sample from a Poisson distribution with mean λ, then

$$P(X_1 = x_1, X_2 = x_2, \dots, X_n = x_n) = p_{X_1, X_2, \dots, X_n}(x_1, x_2, \dots, x_n) = \frac{e^{-n\lambda} \lambda^{\left(\sum_{i=1}^{n} x_i\right)}}{\prod_{i=1}^{n} x_i!}$$

for $\lambda > 0$. See Section 6.4 for derivation.

However, in the study of statistics, we assume the parameter values are **unknown**. Therefore, if we are given a specific random sample $x_1, x_2, \dots, x_n$, then $p(x_1, x_2, \dots, x_n)$ will take on different values for each possible value of the parameters (λ in the Poisson example). Hence, we can consider $p(x_1, x_2, \dots, x_n)$ to also be a function of the unknown parameter and write $p(x_1, x_2, \dots, x_n|\lambda)$ to make the dependence on λ explicit. In **maximum likelihood estimation** we choose $\hat{\lambda}$ to be the value of λ which most likely produced the random sample $x_1, x_2, \dots, x_n$, that is, the value of λ which maximises $p(x_1, x_2, \dots, x_n|\lambda)$ for the observed $x_1, x_2, \dots, x_n$.

Definition 10.3.1. **Likelihood function**

The *likelihood function* of the random variables $X_1, X_2, \dots, X_n$ is the joint p.m.f.

(discrete case) or joint p.d.f. (continuous case) of the observed data given the parameter θ, that is

$$L(\theta) = f(x_1, x_2, \ldots, x_n|\theta).$$

Note that if $X_1, X_2, \ldots, X_n$ are a random sample from a distribution with probability function $f(x|\theta)$ then

$$L(\theta) = \prod_{i=1}^{n} f(x_i|\theta).$$

Definition 10.3.2. **Maximum likelihood estimator**

The *maximum likelihood estimator*, denoted shorthand by MLE or m.l.e., of θ is the value $\hat{\theta}$ which maximises $L(\theta)$.

Example 10.3.3. Suppose that we collect a random sample from a Poisson distribution such that $X_1 = 1$, $X_2 = 2$, $X_3 = 3$ and $X_4 = 4$. Find the maximum likelihood estimator of λ.

The likelihood function is

$$\begin{aligned} L(\lambda) &= p(x_1, x_2, x_3, x_4|\lambda) \\ &= p(1, 2, 3, 4|\lambda) \\ &= \frac{e^{-4\lambda}\lambda^{10}}{1!2!3!4!}. \end{aligned}$$

Since $\log x$ is a monotonic increasing function, the value $\hat{\lambda}$ that maximises $\log L(\lambda)$ will also maximise $L(\lambda)$. Hence calculate,

$$\log L(\lambda) = -4\lambda + 10 \log \lambda - \log(1!2!3!4!).$$

To maximise $\log L(\lambda)$ we solve

$$\frac{d \log L(\lambda)}{d\lambda} = 0.$$

Now, $\frac{d \log L(\lambda)}{d\lambda} = -4 + \frac{10}{\lambda} = 0$. Hence, $\widehat{\lambda} = \frac{5}{2} = 2.5$.

Definition 10.3.4. **Log likelihood function**

If $L(\theta)$ is the likelihood function of θ, then $l(\theta) = \log L(\theta)$ is called the *log likelihood function* of θ.

Example 10.3.5. **Binomial MLE**

Let $X \sim \text{Bin}(m, \theta)$. Find the MLE of θ given observation x.

Attempt Example 10.3.5: Binomial MLE and then watch Video 17 for the solutions.

We will use the case $m = 10$ and $x = 3$ to illustrate the calculations.

Watch Video 17: Binomial MLE

Solution to Example 10.3.5: Binomial MLE

Given x is sampled from the random variable X, we have that

$$L(\theta) = \binom{m}{x} \theta^x (1-\theta)^{m-x}, \qquad 0 \leq \theta \leq 1.$$

In the case $m = 10$ and $x = 3$ the likelihood becomes $L(\theta) = 120\theta^3(1-\theta)^7$ and this is illustrated in Figure 10.1.

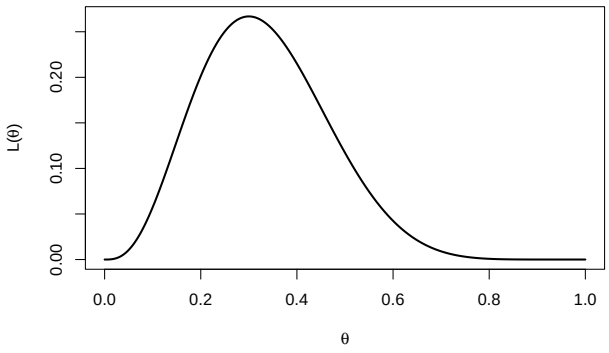


Figure 10.1: Likelihood function.

Take the derivative of $L(\theta)$ (using the product rule):

$$\begin{aligned}\frac{dL(\theta)}{d\theta} &= \binom{m}{x} x\theta^{x-1}(1-\theta)^{m-x} - \binom{m}{x}\theta^{x}(m-x)(1-\theta)^{m-x-1} \\ &= \binom{m}{x}\theta^{x-1}(1-\theta)^{m-x-1}\left[x(1-\theta)-(m-x)\theta\right].\end{aligned}$$

Setting $\frac{dL(\theta)}{d\theta} = 0$, we obtain

$$[x(1-\theta)-(m-x)\theta] = 0.$$

Hence, $\hat{\theta} = \frac{x}{m}$ is a possible value for the MLE of θ.

Since $L(\theta)$ is a continuous function over $[0,1]$, the maximum must exist at either the stationary point or at one of the endpoints of the interval. Given, $L(0) = 0$, $L(1) = 0$, and $L\left(\frac{x}{m}\right) > 0$, it follows that $\hat{\theta} = \frac{x}{m}$ is the MLE of θ.

In the illustrative example, $m = 10$ and $x = 3$ giving $\hat{\theta} = \frac{3}{10} = 0.3$. In Figure 10.2 the MLE is marked on the plot of the likelihood function.

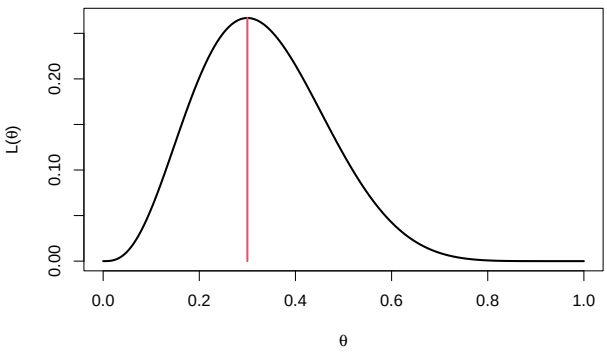


Figure 10.2: Likelihood function with MLE at 0.3.

It is easier to use the log-likelihood $l(\theta)$ to derive the MLE.

We have that

$$l(\theta) = \log\left[\binom{m}{x}\theta^{x}(1-\theta)^{m-x}\right] = \log\left[\binom{m}{x}\right] + x\log\theta + (m-x)\log(1-\theta).$$

In the case $m = 10$ and $x = 3$ the likelihood becomes $l(\theta) = \log 120 + 3\log\theta + 7\log(1-\theta)$ and this is illustrated in Figure 10.3.

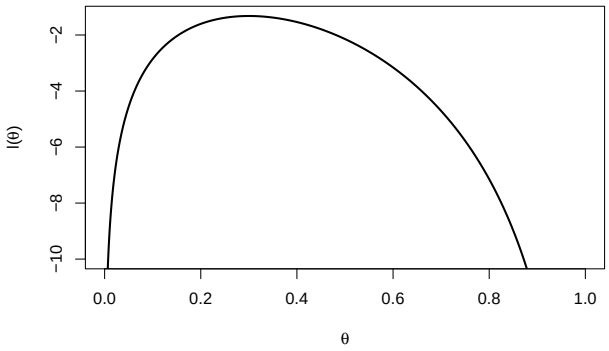


Figure 10.3: Log-likelihood function.

Take the derivative of $l(\theta)$:

$$\begin{aligned}\frac{dl(\theta)}{d\theta} &= 0 + \frac{x}{\theta} - \frac{m-x}{1-\theta} \\ &= \frac{x(1-\theta) - (m-x)\theta}{\theta(1-\theta)}.\end{aligned}$$

Setting $\frac{dl(\theta)}{d\theta} = 0$, again requires solving

$$[x(1-\theta) - (m-x)\theta] = 0.$$

Giving $\hat{\theta} = \frac{x}{m}$.

In the illustrative example, $m = 10$ and $x = 3$ giving $\hat{\theta} = \frac{3}{10} = 0.3$. In Figure 10.4 the MLE is marked on the plot of the likelihood function.

The following **R** shiny app allows you to investigate the MLE for data from a geometric distribution, $X \sim \text{Geom}(p)$. The success probability of the geometric distribution can be varied from 0.01 to 1. The likelihood, log-likelihood and relative likelihood (likelihood divided by its maximum) functions can be plotted. Note that as the number of observations become large the likelihood becomes very small, and equal to, 0 to computer accuracy. You will observe that the likelihood function becomes more focussed about the MLE as the sample size increases. Also the MLE will generally be closer to the *true* value of p used to generate the data as the sample size increases.

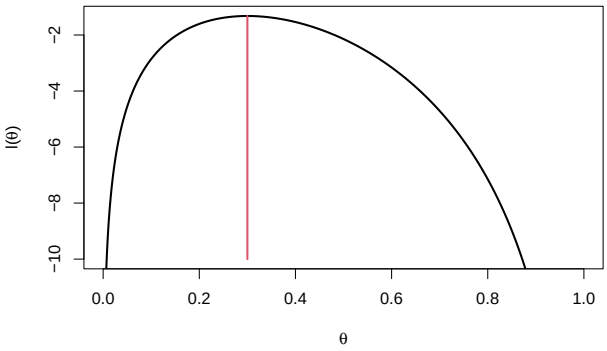


Figure 10.4: Log-likelihood function with MLE at 0.3.

R Shiny app: MLE Geometric Distribution

Example 10.3.6. **Poisson MLE**

Let $X_1, X_2, \ldots, X_n$ be a random sample from a Poisson distribution with mean λ. Find the MLE of λ.

We have

$$\begin{aligned} L(\lambda) &= p(x_1, x_2, \ldots, x_n|\lambda) \\ &= \frac{\mathrm{e}^{-n\lambda}\lambda^{\sum_{i=1}^n x_i}}{\prod_{i=1}^n x_i!}, \end{aligned}$$

where $\lambda > 0$. So,

$$l(\lambda) = -n\lambda + \sum_{i=1}^n x_i \log\lambda - \log\prod_{i=1}^n x_i!.$$

Now

$$\frac{dl(\lambda)}{d\lambda} = -n + \frac{\sum_{i=1}^n x_i}{\lambda}.$$

Setting $\frac{dl(\lambda)}{d\lambda} = 0$ and solving yields

$$\hat{\lambda} = \frac{\sum_{i=1}^{n} x_i}{n} = \bar{x}.$$

Since $\frac{d^2 l(\lambda)}{d\lambda^2} = \frac{-\sum_{i=1}^{n} x_i}{\lambda^2} < 0$, it follows that $\hat{\lambda} = \bar{X}$ is a maximum, so is the MLE of λ.

In both Example 10.3.5 and Example 10.3.6, we note that terms in the likelihood which do not involve the parameter of interest play no role in the calculating of the MLE. For example, $\binom{m}{x}$ in the binomial and $\left[\prod_{i=1}^{n} x_i!\right]^{-1}$ in the Poisson. Therefore it is sufficient to consider a function $H(\theta)$ which is proportional to the likelihood, that is, there exists $K > 0$ such that

$$L(\theta) = KH(\theta) \qquad \text{for all } \theta.$$

We write $L(\theta) \propto H(\theta)$ and note that if $h(\theta) = \log H(\theta)$, then

$$l(\theta) = \log K + h(\theta)$$

and

$$\frac{d}{d\theta} l(\theta) = \frac{d}{d\theta} h(\theta).$$

Example 10.3.7. **MLE of mean of a Normal random variable**

Let $X_1, X_2, \ldots, X_n$ be a random sample of $N(\theta, 1)$ with mean θ. Find the MLE of θ given observations $x_1, x_2, \ldots, x_n$.

For each of the x_i:

$$f(x_i|\theta) = \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2}(x_i - \theta)^2\right\}.$$

Thus:

$$L(\theta) = (2\pi)^{-n/2} \prod_{i=1}^{n} \exp\left\{-\frac{1}{2}(x_i - \theta)^2\right\}$$

and so,

$$L(\theta) \propto \prod_{i=1}^{n} \exp\left\{-\frac{1}{2}(x_i - \theta)^2\right\} = \exp\left\{-\frac{1}{2}\sum_{i=1}^{n}(x_i - \theta)^2\right\}$$

and

$$l(\theta) = \log L(\theta) = -\frac{1}{2}\sum_{i=1}^{n}(x_i - \theta)^2 + \text{constant}.$$

Hence

$$\frac{dl(\theta)}{d\theta} = \sum_{i=1}^{n}(x_i - \theta) = 0$$

gives the stationary point of the likelihood, with

$$\hat{\theta} = \frac{\sum x_i}{n} = \bar{x}, \tag{10.1}$$

It is easily verified that $\hat{\theta}$ given in (10.1) is a maximum since

$$\frac{d^2 l(\theta)}{d\theta^2} = -n < 0.$$

So $\hat{\theta} = \bar{x}$ is the MLE of θ.

In Example 10.3.5, Example 10.3.6 and Example 10.3.7 the maximum likelihood estimators correspond with the method of moment estimators. In Example 10.3.8 we consider a situation where the maximum likelihood estimator is very different from the method of moments estimator.

Example 10.3.8. **MLE for Uniform random variables**

Let $U_1, U_2, \ldots, U_n$ be i.i.d. samples of $U[0, \theta]$. Given observations $u_1, u_2, \ldots, u_n$:

(a) Find the MLE of θ.

(b) Find the method of moments estimator of θ.

Attempt Example 10.3.8: MLE for Uniform random variables and then watch Video 18 for the solutions.

We will data $\mathbf{u} = (u_1, u_2, \dots, u_5) = (1.30, 2.12, 2.40, 0.98, 1.43)$ as an illustrative example. These 5 observations were simulated from $U(0, 3)$.

Watch Video 18: MLE for Uniform random variables

Solution to Example 10.3.8: MLE for Uniform random variables

(a) If $U_i \sim U[0, \theta]$, then its p.d.f. is given by

$$f(u|\theta) = \begin{cases} \frac{1}{\theta}, & \text{if } 0 \leq u \leq \theta, \\ 0, & \text{otherwise.} \end{cases}$$

Note that if $\theta < u_i$ for some i, then $L(\theta) = 0$. Since $L(\theta)$ is always positive and we want to maximise L, we can assume $0 \leq u_i \leq \theta$ for all $i = 1, \dots, n$, then

$$L(\theta) = \prod_{i=1}^{n} f(u_i|\theta) = \prod_{i=1}^{n} \frac{1}{\theta} = \frac{1}{\theta^n}.$$

Hence, $L(\theta)$ is a decreasing function of θ and its maximum must exist at the smallest value that θ can obtain. Since $\theta > \max\{u_1, u_2, \dots, u_n\}$, the MLE of θ is $\hat{\theta} = \max\{u_1, u_2, \dots, u_n\}$.

Figure 10.5 shows the likelihood function $L(\theta)$ using the data $\mathbf{u} = (1.30, 2.12, 2.40, 0.98, 1.43)$.

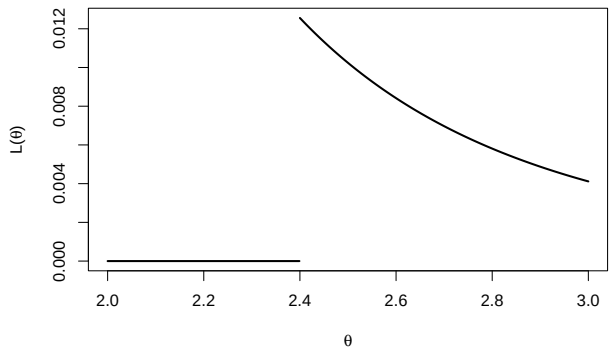


Figure 10.5: Likelihood function for u = (1.30,2.12,2.40,0.98,1.43).

(b) By comparison the method of moments estimator, $\breve{\theta}$, of θ uses $E[U] = \frac{0+\theta}{2}$ and hence is given by

$$\breve{\theta} = 2\bar{u}.$$

Note that if $2\bar{u} < \max\{u_1, u_2, \ldots, u_n\}$ then $\breve{\theta}$ will not be consistent with the data, *i.e.* $L(\breve{\theta}) = 0$.

To observe the difference between the MLE and the method of moments estimator, using $\mathbf{u} = (1.30, 2.12, 2.40, 0.98, 1.43)$:

- MLE: $\hat{\theta} = \max\{1.30, 2.12, 2.40, 0.98, 1.43\} = 2.40$;
- Method of Moments: $\breve{\theta} = 2\bar{u} = 2(1.646) = 3.292$.

10.4 Comments on the Maximum Likelihood Estimator

The following points on the maximum likelihood estimator are worth noting:

1. When finding the MLE you want to maximise the likelihood function. However it is often more convenient to maximise the log likelihood function instead. Both functions will be maximised by the same parameter values;

2. MLEs may not exist, and if they do, they may not be unique;

3. The likelihood function is **NOT** the probability distribution for θ. The correct interpretation of the likelihood function is that it is the probability of obtaining the observed data if θ were the true value of the parameter. We assume θ is an unknown constant, not a random variable. In Bayesian statistics we will consider the parameter to be random;

4. The MLE has some nice large sample properties, including consistency, asymptotic normality and other optimality properties;

5. The MLE can be used for non-independent data or non-identically distributed data as well;

6. Often the MLE cannot be found using calculus techniques and must be found numerically. It is often useful, if we can, to plot the likelihood function to find good starting points to find the MLE numerically;

7. The MLE satisfies a useful invariance property. Namely, if $\phi = h(\theta)$, where $h(\theta)$ is a one-to-one function of θ, then the MLE of ϕ is given by $\hat{\phi} = h(\hat{\theta})$. For example, if $\phi = \frac{1}{\theta}$ and $\hat{\theta} = \bar{X}$ then $\hat{\phi} = \frac{1}{\hat{\theta}} = \frac{1}{\bar{X}}$.

Student Exercises

Attempt the exercises below.

Exercise 10.1.
Let $X_1, X_2, \ldots, X_n$ be independent random variables, each with pdf

$$f(x|\theta) = \theta^2 x \exp(-\theta x),$$

for $x > 0$. Use the method of moments to determine an estimator of θ.

Remember that if $X \sim \text{Gamma}(\alpha, \beta)$ then $E[X] = \alpha/\beta$.

Exercise 10.2.
Let $X_1, X_2, \ldots, X_n$ be a random sample from the distribution with p.d.f.

$$f(x|\theta) = \theta e^{-(x-1)\theta}, \qquad x > 1,$$

where $\theta > 0$ is an unknown parameter. Find the MLE of θ.

Exercise 10.3.
(a) Let $X_1, X_2, \ldots, X_n$ be a random sample from the distribution having pdf

$$f(x|\theta) = \frac{1}{2}(1 + \theta x), \qquad -1 < x < 1,$$

where $\theta \in (-1, 1)$ is an unknown parameter. Show that the method of moments estimator for θ is

$$\tilde{\theta}_1 = 3\bar{X}$$

where $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$.
(b) Suppose instead that it is observed only whether a given observation is positive or negative. For $i = 1, 2, \ldots, n$, let

$$Y_i = \begin{cases} 1 & \text{if } X_i \geq 0 \\ 0 & \text{if } X_i < 0. \end{cases}$$

Show that the method of moments estimator for θ based on $Y_1, Y_2, \ldots, Y_n$ is

$$\tilde{\theta}_2 = 4\bar{Y} - 2,$$

where $\bar{Y} = \frac{1}{n}\sum_{i=1}^{n} Y_i$.
(c) Justifying your answers,

i. which, if either, of the estimators $\tilde{\theta}_1$ and $\tilde{\theta}_2$ are unbiased?

ii. which of the estimators $\tilde{\theta}_1$ and $\tilde{\theta}_2$ is more efficient?

iii. which, if either, of the estimators $\tilde{\theta}_1$ and $\tilde{\theta}_2$ are mean-square consistent?

Chapter 11

Additional Properties of Estimators

11.1 Introduction

In this section, we introduce four key concepts associated with estimators, especially maximum likelihood estimators (MLE):

- Sufficiency
- Minimum variance estimators
- Asymptotic normality of the MLE

- Invariance principle

Sufficiency considers the question of what information from the data, $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ is **sufficient** to estimate a population parameter, θ, without loss of information. Often sufficient statistics will take the form of a summary statistic, for example, the mean.

Minimising the mean square error (MSE) of estimators is a desirable property. For unbiased estimators minimising the variance of the estimator is equivalent to minimising the MSE. We introduce the Cramer-Rao lower bound which is the minimum variance obtainable by an unbiased estimator and the concept of **minimum variance unbiased estimators** (MVUE) as estimators which obtain the Cramer-Rao lower bound.

For large n, the MLE, $\widehat{\theta}$ is approximately normally distributed about the true population parameter θ with variance determined by the second derivative of the likelihood. The variance of the asymptotic normal distribution coincides with the Cramer-Rao lower bound providing further support for using maximum likelihood estimation.

11.2 Sufficiency

Definition 11.2.1. **Sufficient Statistic**

Let $\mathbf{X} = (X_1, X_2, \dots, X_n)$ where $X_1, X_2, \dots, X_n$ are i.i.d. random variables dependent on a parameter θ. A statistic $T(\mathbf{X}) = T$ is **sufficient** for θ if the conditional distribution of $\mathbf{X}|T$ does not depend on θ, that is

$$f(x_1, x_2, \dots, x_n|T = t, \theta) = u(x_1, x_2, \dots, x_n|T = t),$$

where u is a function of $x_1, x_2, \dots, x_n$ only. Thus, T contains all the information about θ.

The key point is that a **sufficient** statistic, as the name suggests, is sufficient for the estimation of a parameter θ. This is particularly useful if the sufficient statistic is a low-dimensional summary statistic of the data. As the following examples show in many cases there is a one-dimensional summary statistic of the data $\mathbf{x} = (x_1, x_2, \dots, x_n)$ which is sufficient to estimate the population parameter of interest, θ. The Neyman-Fisher factorisation criterion provides easy to check conditions for sufficiency.

Theorem 11.2.2. **Neyman-Fisher factorisation criterion**

The statistic $T(\mathbf{X})$ is sufficient for θ if and only if one can factor the likelihood function such that

$$L(\theta) = h(\mathbf{x})g(t, \theta),$$

where $h(\mathbf{x})$ does not depend on θ (whenever $L(\theta) > 0$) and g is a non-negative function of t and θ.

The Neyman-Fisher factorisation criterion is equivalent to the log-likelihood function being expressible in the form:

$$l(\theta) = \log h(\mathbf{x}) + \log g(T(\mathbf{x}), \theta) = H(\mathbf{x}) + G(T(\mathbf{x}), \theta).$$

Then if we differentiate $l(\theta)$ with respect to θ, we have that

$$l'(\theta) = \frac{d}{d\theta} l(\theta) = \frac{d}{d\theta} \{H(\mathbf{x}) + G(T(\mathbf{x}), \theta)\} = \frac{d}{d\theta} G(T(\mathbf{x}), \theta).$$

Setting $l'(\theta) = 0$ and solving to obtain the MLE $\hat{\theta}$ is equivalent to solving

$$\frac{d}{d\theta} G(T(\mathbf{x}), \theta) = 0.$$

We observe that $H(\mathbf{x})$ plays no role in the computation of the MLE and the function $G(\cdot, \cdot)$ is a function of the sufficient statistic, $T(\mathbf{x})$ and θ only.

Example 11.2.3. Let $X_1, X_2, \dots, X_n$ be a random sample from $N(\theta, 1)$. Show that $\bar{X}$ is sufficient for θ.

Consider the likelihood function:

$$\begin{aligned}
L(\theta) &= f(x_1, x_2, \dots, x_n|\theta) \\
&= \prod_{i=1}^{n} \frac{1}{(2\pi)^{1/2}} \exp\left(-\frac{1}{2}(x_i-\theta)^2\right) \\
&= \frac{1}{(2\pi)^{n/2}} \exp\left(-\frac{1}{2}\sum_{i=1}^{n}(x_i-\theta)^2\right) \\
&= (2\pi)^{-n/2} \exp\left(-\frac{1}{2}\sum_{i=1}^{n}(x_i^2 - 2\theta x_i + \theta^2)\right) \\
&= (2\pi)^{-n/2} \exp\left(-\frac{1}{2}\left(\sum_{i=1}^{n} x_i^2 - 2\theta\sum_{i=1}^{n} x_i + n\theta^2\right)\right) \\
&= (2\pi)^{-n/2} \exp\left(-\frac{1}{2}\left(\sum_{i=1}^{n} x_i^2\right)\right) \times \exp\left(-\frac{1}{2}\left(-2\theta n\bar{x} + n\theta^2\right)\right).
\end{aligned}$$

Therefore, letting $h(\mathbf{x}) = (2\pi)^{-n/2} \exp\left(-\frac{1}{2}\left(\sum_{i=1}^{n} x_i^2\right)\right)$ and $g(\bar{X}, \theta) = \exp\left(-\frac{1}{2}\left(-2\theta n\bar{x} + n\theta^2\right)\right)$ we can factor the likelihood function. So, by the Neyman-Fisher factorisation criterion, $\bar{X}$ is a sufficient statistic for θ.

Remember in Section 10.3, Example 10.3.7, we have shown that the sample mean is the MLE of θ for $N(\theta, 1)$.

Example 11.2.4.
Let $X_1, X_2, \dots, X_n$ be i.i.d. random variables from a Poisson distribution with parameter λ. Show that $\bar{X}$ is a sufficient statistic for λ using the Neyman-Fisher factorisation criterion.

Consider

$$\begin{aligned}
L(\lambda) &= f(x_1, x_2, \dots, x_n|\lambda) \\
&= \prod_{i=1}^{n} \frac{e^{-\lambda}\lambda^{x_i}}{x_i!} \\
&= \frac{e^{-n\lambda}\lambda^{\sum_{i=1}^{n} x_i}}{\prod_{i=1}^{n} x_i!} \\
&= \frac{1}{\prod_{i=1}^{n} x_i!} e^{-n\lambda}\lambda^{n\bar{x}}.
\end{aligned}$$

If we let $h(\mathbf{x}) = \left\{ \prod_{i=1}^{n} x_i! \right\}^{-1}$ and $g(\bar{X}, \theta) = e^{-n\lambda}\lambda^{n\bar{x}}$, then we have factorised the likelihood function according to the Neyman-Fisher factorisation criterion. So, $\bar{X}$ must be a sufficient statistic of λ.

Note that

- Generally we prefer to use a sufficient statistic as an estimator for θ since the sufficient statistic uses all of the sample information to estimate θ.
- Sufficient statistics always exist, since $T(\mathbf{X}) = (X_1, X_2, \ldots, X_n)$ is itself a sufficient statistic. However, we would prefer a statistic that has as low a dimension as possible. A sufficient statistic with the lowest possible dimensionality is called a *minimal sufficient statistic*.
- The MLE, if it exists, will always be a function of a sufficient statistic.

11.3 Minimum variance estimators

Given a population parameter does there exist a best estimator in general?

Recall that in our previous discussions in Section 9.3 on qualities of estimators we said we would prefer an estimator with as small an MSE as possible. Unfortunately, if we consider the class of all estimators for a particular parameter, there does not exist such an optimality criterion. If we decide to limit ourselves to particular classes of estimators then there do exist certain optimality criterion.

Let's constrain ourselves to the class of unbiased estimators. Suppose that the random variables and their distributions satisfy the following regularity conditions:

- The range of the random variables does not depend on θ. The random variable $X \sim U(0, \theta)$ is an example that does not satisfy this condition.
- The likelihood function is sufficiently smooth to allow us to interchange the operations of differentiation and integration.
- The second derivatives of the log-likelihood function exists.

Theorem 11.3.1. **Cramér-Rao inequality**

Under the above regularity conditions if $T(\mathbf{X})$ is an unbiased estimator of θ, then

$$var(T(\mathbf{X})) \geq \frac{1}{I(\theta)},$$

where $I(\theta) = E\left[-\frac{d^2 l(\theta)}{d\theta^2}\right]$.

Definition 11.3.2. **Fisher's information**

$I(\theta)$ is called the *expected information* or *Fisher's information*.

Definition 11.3.3. **Cramér-Rao lower bound**

$\frac{1}{I(\theta)}$ is called the *Cramér-Rao lower bound*.

The Cramér-Rao inequality implies that the smallest the variance of any unbiased estimator can become is $1/I(\theta)$.

Definition 11.3.4. **Minimum variance unbiased estimator (MVUE)**

If any unbiased estimator $T(\mathbf{X})$ is such that $\text{Var}(T(\mathbf{X})) = 1/I(\theta)$, then we say that $T(\mathbf{X})$ is a **minimum variance unbiased estimator** (MVUE) as no other unbiased estimator will be able to obtain a smaller variance.

Example 11.3.5. Suppose $X_1, X_2, \ldots, X_n$ are i.i.d. random variables from a Poisson distribution with parameter λ. Does the maximum likelihood estimator $\hat{\lambda} = \bar{X}$ achieve the Cramér-Rao lower bound?

Firstly note that

$$E[\bar{X}] = \frac{1}{n}\sum_{i=1}^{n} E[X_i] = \frac{1}{n}\sum_{i=1}^{n} \lambda = \lambda.$$

Therefore $\bar{X}$ is an unbiased estimator. Now

$$L(\lambda) = \frac{e^{-n\lambda}\lambda^{\sum_{i=1}^{n} x_i}}{\prod_{i=1}^{n} x_i!}.$$

This implies,

$$l(\lambda) = -n\lambda + \sum_{i=1}^{n} x_i \log\lambda - \log\left(\prod_{i=1}^{n} x_i!\right).$$

Therefore,

$$\frac{dl(\lambda)}{d\lambda} = -n + \frac{\sum_{i=1}^{n} x_i}{\lambda},$$
$$\frac{d^2l(\lambda)}{d\lambda^2} = -\frac{\sum_{i=1}^{n} x_i}{\lambda^2}.$$

Computing Fisher's information,

$$\begin{aligned} I(\lambda) &= E\left[-\frac{d^2l(\lambda)}{d\lambda^2}\right] \\ &= E\left[-\left(-\frac{\sum_{i=1}^{n} X_i}{\lambda^2}\right)\right] \\ &= \frac{\sum_{i=1}^{n} E[X_i]}{\lambda^2} \\ &= \frac{n\lambda}{\lambda^2} \\ &= \frac{n}{\lambda}. \end{aligned}$$

Hence, according to the Cramér-Rao inequality,

$$\text{Var}(\bar{X}) \geq \frac{1}{I(\lambda)} = \frac{\lambda}{n}.$$

Now, since $X_i \sim \text{Poi}(\lambda)$, $\text{Var}(\bar{X}) = \frac{\lambda}{n}$. Therefore, $\bar{X}$ is a MVUE for λ.

11.4 Asymptotic normality of the MLE

Theorem 11.4.1. **Asymptotic normality of the MLE**

If $\hat{\theta}$ is the MLE of θ, then under certain regularity conditions it can be shown that

$$\sqrt{n}(\hat{\theta} - \theta) \longrightarrow N\left(0, \frac{n}{I(\theta)}\right), \qquad \text{as } n \to \infty.$$

Hence, approximately for sufficiently large sample sizes,

$$\hat{\theta} \sim N\left(\theta, \frac{1}{I(\theta)}\right).$$

As a consequence the MLE has the following asymptotic properties:

- $\hat{\theta}$ is asymptotically unbiased;
- $\hat{\theta}$ is asymptotically fully efficient, that is the variance of $\hat{\theta}$ approaches the Cramér-Rao lower bound:

$$\text{Var}(\hat{\theta}) \to I(\theta)^{-1}, \qquad \text{as } n \to \infty;$$

- $\hat{\theta}$ is asymptotically normally distributed.

Despite the fact that $var(\hat{\theta}) \approx \frac{1}{I(\theta)}$ for large n, when θ is unknown then $I(\theta)$ is also unknown. Consequently, if we need to know the variance we may need to estimate it as well. To do this it may be convenient to replace the expected information $I(\theta)$ with the observed Fisher information

$$I_O(\hat{\theta}) = -\frac{d^2 l(\theta)}{d\theta^2}\bigg|_{\theta=\hat{\theta}}.$$

Although the asymptotic properties of the MLE are quite good, the properties are only true for sufficiently large samples. The properties do not necessarily hold for small samples and for any finite sample they are approximations. The asymptotic normality of the MLE is an example of the Central Limit Theorem, and consequently the quality of the approximation will depend on the underlying distribution.

11.5 Invariance property

If $\phi = g(\theta)$, where g is one-to-one monotonic function of θ, then $\hat{\phi} = g(\hat{\theta})$ is the MLE of ϕ, and for large n:

$$\hat{\phi} \approx N\left(\phi, \frac{[g'(\theta)]^2}{I(\theta)}\right),$$

where $g'(\theta) = \frac{d}{d\theta} g(\theta)$.

Note that for $\hat{\phi} = g(\hat{\theta})$ to be the MLE of ϕ it is not necessary for g to be strictly one-to-one. It is sufficient for the range of g to be an interval.

Example 11.5.1. **Properties of Poisson MLE**

Let $X_1, X_2, \ldots, X_n$ be a random sample from a Poisson distribution with parameter λ. We have shown $\hat{\lambda} = \bar{X}$ is the MLE of λ.

(a) What is its asymptotic distribution?

(b) Compute $p = P(X_1 = 0)$.

(c) Find the MLE for $P(X_1 = 0)$ and its asymptotic distribution.

(d) An alternative approach to estimate $p = P(X_1 = 0)$ is the proportion of observations $X_1, X_2, \ldots, X_n$ which are equal to 0,

$$\tilde{p} = \frac{1}{n}\sum_{i=1}^{n} I(X_i = 0),$$

where $I(A) = 1$ if the event A occurs and 0 otherwise. Show that $\tilde{p}$ is unbiased and find its asymptotic distribution.

Attempt Example 11.5.1: Properties of Poisson MLE and then watch Video 19 for the solutions.

Watch Video 19: Properties of Poisson MLE

Solution to Example 11.5.1: MLE for Properties of Poisson MLE.

(a) According to the Asymptotic normality of the MLE Theorem, since $\hat{\lambda}$ is the MLE of λ, then $\hat{\lambda} \to N\left(\lambda, \frac{1}{I(\lambda)}\right)$. We have shown that $I(\lambda) = \frac{n}{\lambda}$, therefore, $\hat{\lambda} \to N\left(\lambda, \frac{\lambda}{n}\right)$.

(b) We calculate

$$p = P(X_1 = 0) = \frac{e^{-\lambda}\lambda^0}{0!} = e^{-\lambda}.$$

(c) Set $p = P(X_1 = 0) = e^{-\lambda} = g(\lambda)$. Then since the range of g is an interval, specifically $(0, \infty)$, the MLE of p is given by

$$\hat{p} = g(\hat{\lambda}) = e^{-\hat{\lambda}} = e^{-\bar{X}}.$$

By the invariance property,

$$\hat{p} \to N\left(p, \frac{[g'(\lambda)]^2}{I(\lambda)}\right),$$

where $g'(\lambda) = -e^{-\lambda}$. Therefore $\hat{p} \to N\left(p, \frac{e^{-2\lambda}}{n/\lambda}\right)$. Using $p = e^{-\lambda}$, then $\lambda = -\log(p)$ and by substitution

$$\hat{p} \to N\left(p, \frac{-p^2\log(p)}{n}\right), \qquad \text{as } n \to \infty.$$

(d) For an event A the function $1_{\{A\}}$ (known as the indicator function of A) takes the value 1 if A occurs and 0 otherwise. Thus $E[1_{\{A\}}] = P(A)$, the expectation for how likely the event A is to occur is simply the probability that the event A occurs. Compare with the Bernoulli distribution.
Therefore

$$\begin{aligned} E[\tilde{p}] &= E\left[\frac{1}{n}\sum_{i=1}^{n} 1_{\{X_i=0\}}\right] \\ &= \frac{1}{n}\sum_{i=1}^{n} E[1_{\{X_i=0\}}] \\ &= \frac{1}{n} nP(X_1 = 0) = p, \end{aligned}$$

and $\tilde{p}$ is an unbiased estimator.
Moreover, if $Y = \sum_{i=1}^{n} 1_{\{X_i=0\}}$, the number of observations equal to 0, then $Y \sim \text{Bin}(n, p)$. For large n, the Central Limit Theorem (Section 7.2) states $Y \approx N(np, np(1-p))$ and hence

$$\tilde{p} = \frac{Y}{n} \approx N\left(p, \frac{p(1-p)}{n}\right).$$

Comparing the asymptotic variances of $\hat{p}$ and $\tilde{p}$ as $p = \exp(-\lambda)$ varies in Figure 11.1 we note that the asymptotic variance of $\hat{p}$ is always smaller. That is, it is better to use information about the whole distribution ($\bar{X}$) rather than simply which observations are equal to 0 and those which are not. Note that as $p \to 1$ corresponding to $\lambda \to 0$ the difference between the variances becomes smaller.

Task: Session 6

Attempt the **R Markdown** file for Session 6:
Session 6: Properties of MLEs

Student Exercises

Attempt the exercises below.

Exercise 11.1.
Consider the situation where Bernoulli trials are available. The number of trials required before 5 successes are obtained can be modelled by the negative

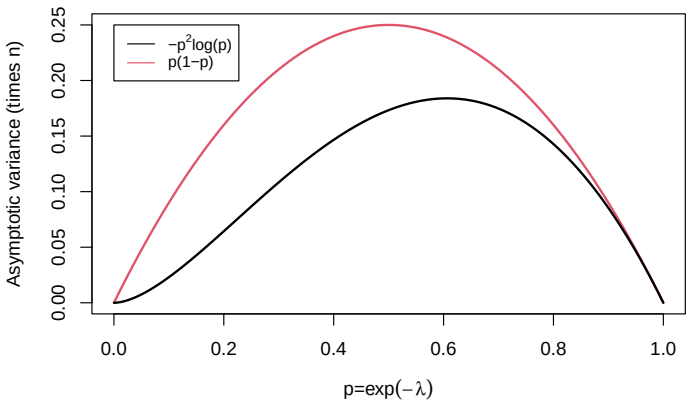


Figure 11.1: Asymptotic variance times sample size, n, for varying p.

binomial distribution with parameters $r = 5$ and θ. The probability mass function of a negative binomial is:

$$p(x) = \binom{x-1}{r-1}\theta^r(1-\theta)^{x-r}, \qquad x = r, r+1, \ldots .$$

Find the maximum likelihood estimator $\hat{\theta}$ of θ based on a random sample of n sets of trials. What are the maximum likelihood estimators of:
(a) the mean of the distribution $5/\theta$, and,
(b) the quantity θ^5?

Exercise 11.2.
To determine the amount that a particular type of bacteria is present in water one finds out whether or not *any* is present in multiple samples. Let θ be the average number of bacteria per unit volume in the river, and assume that the bacteria are distributed at random in the water. Some n test tubes each containing a volume v of river water are incubated and tested. A negative test shows no bacteria whereas a positive test shows that at least one bacterium is present. If y tubes out of n tested give negative results, what is the m.l.e. of θ?

Chapter 12

Conditional Distribution and Conditional Expectation

In this section, we consider further the joint behaviour of two random variables X and Y, and in particular, studying the conditional distribution of one random variable given the other. We start with discrete random variables and then move onto continuous random variables.

12.1 Conditional distribution

Recall that for any two events E and F such that $P(F) > 0$, we defined in Section 4.6 that

$$P(E|F) = \frac{P(E \cap F)}{P(F)}.$$

Can we extend this idea to random variables?

Definition 12.1.1. **Conditional p.m.f.**

If X and Y are discrete random variables, the *conditional probability mass function* of X given $Y = y$ is

$$\begin{aligned} p_{X|Y}(x|y) &= P(X = x|Y = y) \\ &= \begin{cases} \frac{p_{X,Y}(x,y)}{p_Y(y)} & \text{if } p_Y(y) > 0 \\ 0 & \text{otherwise.} \end{cases} \end{aligned}$$

where $p_{X,Y}(x,y)$ is the joint p.m.f. of X and Y and $p_Y(y)$ is the marginal p.m.f. of Y for any x and y such that $p_Y(y) > 0$.

Note that

- Conditional probabilities are non-negative:

$$P(X = x|Y = y) = \frac{p_{X,Y}(x,y)}{p_Y(y)} \geq 0.$$

- The sum of conditional probabilities over all values of x for some fixed value of y is 1:

$$\begin{aligned}\sum_x P(X = x|Y = y) &= \sum_x \frac{p_{X,Y}(x,y)}{p_Y(y)} \\ &= \frac{1}{p_Y(y)} \sum_x p_{X,Y}(x,y) \\ &= \frac{1}{p_Y(y)} p_Y(y) \\ &= 1.\end{aligned}$$

  This implies that $P(X = x|Y = y)$ is itself a p.m.f.

Definition 12.1.2. **Conditional c.d.f. (discrete random variable)**

If X and Y are discrete random variables, the *conditional (cumulative) probability distribution function* of X given $Y = y$ is

$$F_{X|Y}(x|y) = P(X \leq x|Y = y) = \sum_{x' \leq x} p_{X|Y}(x'|y).$$

Example 12.1.3.
Suppose the joint p.m.f. of X and Y is given by the following probability table.

X/Y	y=0	y=1	y=2	y=3
x=0	0	$\frac{1}{42}$	$\frac{2}{42}$	$\frac{3}{42}$
x=1	$\frac{2}{42}$	$\frac{3}{42}$	$\frac{4}{42}$	$\frac{5}{42}$
x=2	$\frac{4}{42}$	$\frac{5}{42}$	$\frac{6}{42}$	$\frac{7}{42}$

Determine the conditional p.m.f. of Y given $X = 1$.

$$p_{Y|X}(y|x = 1) = \frac{p_{X,Y}(x = 1, y)}{p_X(x = 1)} = \frac{p_{X,Y}(x = 1, y)}{14/42}.$$

The conditional p.m.f. of Y given $X = 1$ is therefore

$$p_{Y|X}(y|x=1) = \begin{cases} \frac{2/42}{14/42} = \frac{2}{14}, & \text{if } y = 0, \\ \frac{3/42}{14/42} = \frac{3}{14}, & \text{if } y = 1, \\ \frac{4/42}{14/42} = \frac{4}{14}, & \text{if } y = 2, \\ \frac{5/42}{14/42} = \frac{5}{14}, & \text{if } y = 3. \end{cases}$$

We cannot extend this idea to the continuous case directly since for a continuous random variable Y, and for any fixed value y, one has $P_Y(Y = y) = 0$.

Definition 12.1.4. **Conditional p.d.f.**

If X and Y have a joint p.d.f. $f_{X,Y}$, then the *conditional probability density function* of X, given that $Y = y$, is defined by

$$f_{X|Y}(x|y) = \begin{cases} \frac{f_{X,Y}(x,y)}{f_Y(y)}, & \text{if } f_Y(y) > 0, \\ 0, & \text{otherwise.} \end{cases}$$

Definition 12.1.5. **Conditional c.d.f. (continuous random variable)**

Furthermore, we can define the *conditional (cumulative) probability distribution function* of X, given $Y = y$, as

$$F_{X|Y}(x|y) = P(X \leq x|Y = y) = \int_{-\infty}^{x} f_{X|Y}(u|y)du.$$

Example 12.1.6.
Suppose that the joint p.d.f. of X and Y is given by

$$f_{X,Y}(x,y) = \begin{cases} 24x(1-x-y), & \text{if } x \geq 0, y \geq 0, x+y \leq 1, \\ 0, & \text{otherwise.} \end{cases}$$

Find

(a) the conditional p.d.f. of X given $Y = y$;

(b) the conditional p.d.f. of X given $Y = \frac{1}{2}$.

(a) In Section 6.2, Example 6.2.3, we found

$$f_Y(y) = \begin{cases} 4(1-y)^3, & 0 \le y \le 1, \\ 0, & \text{otherwise.} \end{cases}$$

Therefore,

$$\begin{aligned} f_{X|Y}(x|y) &= \frac{f_{X,Y}(x,y)}{f_Y(y)} \\ &= \begin{cases} \frac{24x(1-x-y)}{4(1-y)^3}, & \text{if } x \ge 0, y \ge 0, x+y \le 1, \\ 0, & \text{otherwise.} \end{cases} \end{aligned}$$

(b) Therefore setting $y = 1/2$,

$$\begin{aligned} f_{X|Y}\left(x \middle| \frac{1}{2}\right) &= \frac{f_{X,Y}(x, \frac{1}{2})}{f_Y(\frac{1}{2})} \\ &= \begin{cases} \frac{24x(1/2-x)}{4(1/2)^3} = 48x\left(\frac{1}{2}-x\right), & \text{if } 0 \le x \le \frac{1}{2} \\ 0, & \text{otherwise.} \end{cases} \end{aligned}$$

Note that conditional pdf's are themselves pdf's and have all the properties associated with pdf's.

12.2 Conditional expectation

Definition 12.2.1. **Conditional Expectation**

The *conditional expectation* of X, given $Y = y$, is defined by

$$E[X|Y=y] = \begin{cases} \sum\limits_x x p_{X|Y}(x|y), & \text{if } X \text{ is discrete,} \\ \int_{-\infty}^{\infty} x f_{X|Y}(x|y)\, dx, & \text{if } X \text{ is continuous.} \end{cases}$$

Since $f_{X|Y}(x|y) = \frac{f_{X,Y}(x,y)}{f_Y(y)}$, then $f_{X,Y}(x,y) = f_{X|Y}(x|y) f_Y(y)$. Consequently, we can reconstruct the joint p.d.f. (p.m.f.) if we are given either:

- the conditional p.d.f. (p.m.f.) of X given $Y = y$ and the marginal p.d.f. (p.m.f.) of Y;
- the conditional p.d.f. (p.m.f.) of Y given $X = x$ and the marginal p.d.f. (p.m.f.) of X.

Example 12.2.2.
Suppose that the joint p.d.f. of X and Y is given by

$$f_{X,Y}(x,y) = \begin{cases} e^{-(\frac{x}{y}+y)}y^{-1} & 0 < x, y < \infty, \\ 0 & \text{otherwise.} \end{cases}$$

For $y > 0$, find

(a) $P(X > 1|Y = y)$;

(b) $E[X|Y = y]$.

Attempt Example 12.2.2 and then watch Video 20 for the solutions.

Watch Video 20: Conditional Distribution and Expectation

Solution to Example 12.2.2.

(a) For $y > 0$,

$$\begin{aligned} f_Y(y) &= \int_{-\infty}^{\infty} f_{X,Y}(x,y)\,dx \\ &= \int_0^{\infty} e^{-(\frac{x}{y}+y)}y^{-1}\,dx \\ &= y^{-1}e^{-y}\left[-\frac{1}{y}e^{-\frac{x}{y}}\right]_0^{\infty} \\ &= e^{-y} \end{aligned}$$

That is, the marginal distribution of Y is $Y \sim \text{Exp}(1)$.
Hence, for $y > 0$,

$$\begin{aligned} f_{X|Y}(x|y) &= \frac{f_{X,Y}(x,y)}{f_Y(y)} \\ &= \begin{cases} e^{-x/y}y^{-1} & \text{if } x > 0, \\ 0, & \text{if } x \le 0. \end{cases} \end{aligned}$$

Therefore the conditional distribution of $X|Y = y$ is $\text{Exp}(1/y)$.
Thus,

$$\begin{aligned} P(X > 1|Y = y) &= \int_1^\infty f_{X|Y}(x|y)\,dx \\ &= \int_1^\infty e^{-x/y} y^{-1}\,dx \\ &= e^{-1/y}, \end{aligned}$$

which is the probability an $\text{Exp}(1/y)$ random variable takes a value greater than 1.

(b) Furthermore

$$\begin{aligned} E[X|Y = y] &= \int_{-\infty}^\infty x f_{X|Y}(x|y)\,dx \\ &= \int_0^\infty \frac{x}{y} e^{-x/y}\,dx \\ &= y. \end{aligned}$$

As expected since if $W \sim \text{Exp}(1/\theta)$, then $E[W] = \theta$.

In Example 12.2.2, we can write down the joint distribution of X and Y as

$$\begin{aligned} &Y \sim \text{Exp}(1); \\ &X|Y = y \sim \text{Exp}(1/y). \end{aligned}$$

Many joint distributions are constructed in a similar manner, the marginal distribution of the first random variable along with the conditional distribution of the second random variable with respect to the first random variable. Such constructions are particularly common in Bayesian statistics. It enables us to understand key properties of the distribution such as conditional means and also to simulate values from the joint distribution.

The marginal distribution of X does not take a nice form with $f_X(x) \to \infty$ as $x \downarrow 0$, see Figure 12.1.

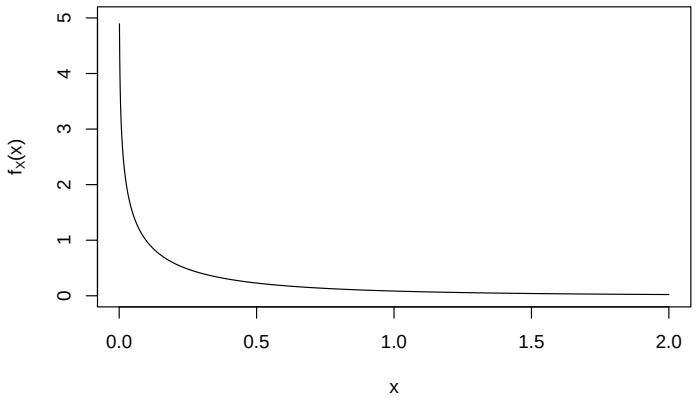


Figure 12.1: Plot of the p.d.f. of X.

We consider the link between the conditional expectation of X given Y and the expectation of (the marginal distribution of) X.

Theorem 12.2.3. **Tower Property.**

Let X and Y be a continuous bivariate distribution with joint p.d.f., $f_{X,Y}(x,y)$. Then

$$E[X] = \int_{-\infty}^{\infty} E[X|Y=y] f_Y(y)\, dy.$$

Note that

$$\begin{aligned} E[X] &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} x f_{X,Y}(x,y)\, dx\, dy \\ &= \int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty} x f_{X|Y}(x|y) f_Y(y)\, dx\right] dy \\ &= \int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty} x f_{X|Y}(x|y)\, dx\right] f_Y(y)\, dy \\ &= \int_{-\infty}^{\infty} E[X|Y=y] f_Y(y)\, dy, \end{aligned}$$

as required.

Therefore in Example 12.2.2,

$$\begin{aligned} E[X] &= \int_{-\infty}^{\infty} E[X|Y=y] f_Y(y)\, dy, \\ &= \int_{0}^{\infty} y f_Y(y)\, dy \\ &= E[Y] = 1. \end{aligned}$$

This is far simpler than trying to obtain the marginal distribution of X to compute $E[X]$.

12.3 Independent random variables

Recall the definition of independence for random variables given in Section 6.4. If X and Y are independent continuous random variables, then for any y such that $f_Y(y) > 0$:

$$f_{X|Y}(x|y) = \frac{f_{X,Y}(x,y)}{f_Y(y)} = \frac{f_X(x) f_Y(y)}{f_Y(y)} = f_X(x), \qquad \text{for all } x \in \mathbb{R}.$$

Student Exercise

Attempt the exercise below.

Exercise 12.1.
Suppose that the joint probability density function of X and Y is

$$f_{X,Y}(x,y) = \begin{cases} 3y(x + \frac{1}{4}y) & 0 \le x, y \le 1 \\ 0 & \text{otherwise.} \end{cases}$$

Find

(a) the conditional probability density function of X given $Y = y$, where $y \in (0, 1]$,

(b) $E[X|Y = y]$, for $y \in (0, 1]$,

(c) $P(X > \frac{1}{2}|Y = 1)$.

Chapter 13

Expectation, Covariance and Correlation

In this section, we study further properties of expectations of random variables. We move on from the expectation of a single random variable to consider the expectation of the function of a collection of random variables, $X_1, X_2, \dots, X_n$. We pay particular attention to the expectation of functions of two random variables X and Y, say. We define the **covariance** as a measure of how the random variables X and Y vary together and the **correlation** which provides a measure of linear dependence between two random variables X and Y.

13.1 Expectation of a function of random variables

Definition 13.1.1.
If $X_1, X_2, \dots, X_n$ are jointly continuous, then the **expectation of the function** $g(X_1, X_2, \dots, X_n)$ is given by

$$E[g(X_1, \dots, X_n)] = \int \cdots \int_{\mathbb{R}^n} g(x_1, \dots, x_n) f_{X_1,\dots,X_n}(x_1, \dots, x_n)\, dx_1 \cdots dx_n$$

Note that if $X_1, X_2, \dots, X_n$ are discrete, we replace the integrals by summations and the joint p.d.f. with the joint p.m.f.

Expectation has the following important properties:

- The expectation of a sum is equal to the sum of the expectations (see Section 5.3):

$$E\left[\sum_{i=1}^{n} X_i\right] = \sum_{i=1}^{n} E[X_i];$$

- If X and Y are **independent**, then

$$E[XY] = E[X]E[Y];$$

- If X and Y are **independent** and g and h are any real functions, then

$$E[g(X)h(Y)] = E[g(X)]E[h(Y)].$$

13.2 Covariance

Definition 13.2.1. **Covariance**

The *covariance* of two random variables, X and Y, is defined by

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

Covariance has the following important properties:

- Covariance is equal to the expected value of the product minus the product of the expected values.

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

- If X and Y are independent, then $cov(X, Y) = 0$. The converse is **NOT** true.

- The covariance of two equal random variables is equal to the variance of that random variable.

$$\text{Cov}(X, X) = \text{Var}(X).$$

- The covariance of a scalar multiple of a random variable (in either argument) is equal to the scalar multiple of the covariance. Additionally covariance is invariant under the addition of a constant in either argument.

$$\text{Cov}(aX + b, cY + d) = ac\text{Cov}(X, Y).$$

- The covariance of a linear combination of random variables is equal to a linear combination of the covariances.

$$\text{Cov}\left(\sum_{i=1}^{m} a_i X_i, \sum_{j=1}^{n} b_j Y_j\right) = \sum_{i=1}^{m}\sum_{j=1}^{n} a_i b_j \text{Cov}(X_i, Y_j).$$

- There is a further relationship between variance and covariance:

$$\text{Var}(X+Y) = \text{Var}(X) + \text{Var}(Y) + 2\text{Cov}(X,Y).$$

- More generally this relationship between variance and covariance becomes:

$$\text{Var}\left(\sum_{i=1}^{n} a_i X_i\right) = \sum_{i=1}^{n} a_i^2 \text{Var}(X_i) + 2\sum_{1\le i<j\le n} a_i a_j \text{Cov}(X_i, X_j).$$

- Consider the above identity if $X_1, X_2, \ldots, X_n$ are independent, and each a_i is equal to 1 (see Section 5.3). Then we have:

$$\text{Var}\left(\sum_{i=1}^{n} X_i\right) = \sum_{i=1}^{n} \text{Var}(X_i).$$

Example 13.2.2. **Density on a circle**

Suppose that X and Y have joint probability density function

$$f_{X,Y}(x,y) = \begin{cases} \frac{1}{\pi} & x^2+y^2 \le 1 \\ 0 & \text{otherwise.} \end{cases}$$

Then $\text{Cov}(X,Y) = 0$ but X and Y are not independent.

Watch Video 21 for an explanation of Example 13.2.2: Density on a circle or see the written explanation below.

Watch Video 21: Density on a circle

Explanation - Example 13.2.2: Density on a circle.

We begin by computing $E[X]$, $E[Y]$ and $E[XY]$.
To compute $E[X]$, we first find $f_X(x)$.
Note that if $X = x$, then

$$x^2+y^2 \le 1 \quad \Leftrightarrow \quad y^2 \le 1-x^2 \quad \Leftrightarrow \quad -\sqrt{1-x^2} \le y \le \sqrt{1-x^2}.$$

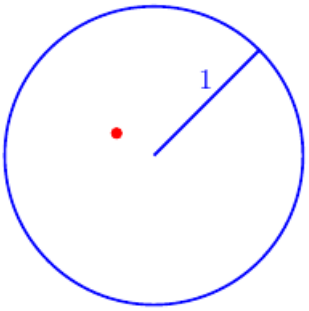


Figure 13.1: Example: Point at $(x, y) = (-0.25, 0.15)$.

Hence, for $-1 < x < 1$,

$$\begin{aligned} f_X(x) &= \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} f_{X,Y}(x,y)\,dy \\ &= \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} \frac{1}{\pi}\,dy \\ &= \left[\frac{y}{\pi}\right]_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} \\ &= \frac{\sqrt{1-x^2}}{\pi} - \frac{-\sqrt{1-x^2}}{\pi} = \frac{2\sqrt{1-x^2}}{\pi}. \end{aligned}$$

Thus

$$f_X(x) = \begin{cases} \frac{2\sqrt{1-x^2}}{\pi} & -1 < x < 1 \\ 0 & \text{otherwise.} \end{cases}$$

see Figure 13.2.

Therefore $E[X]$ is given by

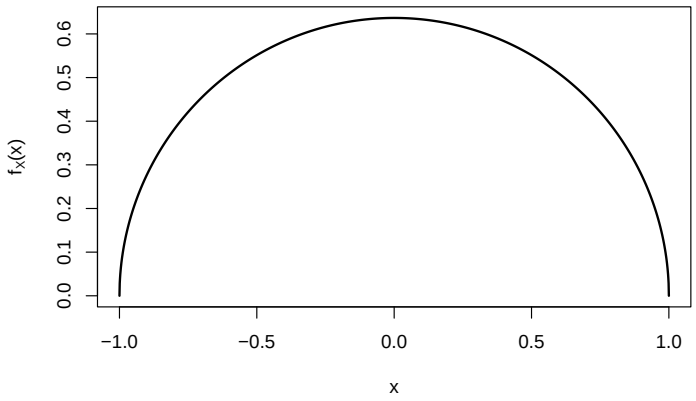


Figure 13.2: Plot of the p.d.f. of X.

$$\begin{aligned} E[X] &= \int_{-\infty}^{\infty} x f_X(x)\,dx \\ &= \int_{-1}^{1} x\frac{2\sqrt{1-x^2}}{\pi}\,dx \\ &= \int_{-1}^{0} x\frac{2\sqrt{1-x^2}}{\pi}\,dx + \int_{0}^{1} x\frac{2\sqrt{1-x^2}}{\pi}\,dx \end{aligned}$$

Using a change of variable $v = -x$ in the first integral:

$$\begin{aligned} \int_{-1}^{0} x\frac{2\sqrt{1-x^2}}{\pi}\,dx &= \int_{1}^{0} (-v)\frac{2\sqrt{1-(-v)^2}}{\pi}\,(-dv) \\ &= -\int_{0}^{1} v\frac{2\sqrt{1-(v)^2}}{\pi}\,dv. \end{aligned}$$

Hence, the red and blue integrals below are equal:

$$\begin{aligned} E[X] &= -\int_{0}^{1} v\frac{2\sqrt{1-v^2}}{\pi}\,dv + \int_{0}^{1} x\frac{2\sqrt{1-x^2}}{\pi}\,dx \\ &= 0. \end{aligned}$$

A symmetry argument gives that

$$f_Y(y) = \begin{cases} \frac{2\sqrt{1-y^2}}{\pi} & -1 < y < 1 \\ 0 & \text{otherwise,} \end{cases}$$

and $E[Y] = 0$.
Now

$$\begin{aligned} E[XY] &= \int\int_{x^2+y^2 \le 1} xy \frac{1}{\pi}\, dy\, dx \\ &= \int_{-1}^{1} \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} xy \frac{1}{\pi}\, dy\, dx \\ &= \int_{-1}^{1} \frac{x}{\pi} \left[\frac{y^2}{2}\right]_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} dx \\ &= \int_{-1}^{1} \frac{x}{2\pi} \left[1 - x^2 - (1-x^2)\right]\, dx \\ &= \int_{-1}^{1} \frac{x}{2\pi}(0)\, dx = 0. \end{aligned}$$

Therefore

$$cov(X, Y) = E[XY] - E[X]E[Y] = 0 - 0 \times 0 = 0.$$

However, X and Y are **not independent**.
Note that for $x = 0.8$ and $y = 0.8$, $x^2 + y^2 = 0.8^2 + 0.8^2 = 1.28 > 1$, so

$$f_{X,Y}(0.8, 0.8) = 0.$$

However, $f_X(0.8) = \frac{2}{\pi}\sqrt{1 - 0.8^2} = 0.382$ and also $f_Y(0.8) = 0.382$ giving

$$f_X(0.8) f_Y(0.8) = 0.382 \times 0.382 \neq 0 = f_{X,Y}(0.8, 0.8).$$

13.3 Correlation

Definition 13.3.1. **Correlation**

If $\text{Var}(X) > 0$ and $\text{Var}(Y) > 0$, then the *correlation* of X and Y is defined by

$$\rho(X,Y) = \frac{\text{Cov}(X,Y)}{\sqrt{\text{Var}(X)\text{Var}(Y)}}.$$

Correlation has the following important properties:

- $-1 \leq \rho(X,Y) \leq 1$.
- If X and Y are independent, then $\rho(X,Y) = 0$. Note, again, that the converse is not true.
- Correlation is invariant under a scalar multiple of a random variable (in either argument) up to a change of sign. Additionally correlation is invariant under the addition of a constant in either argument.

$$\rho(aX+b, cY+d) = \begin{cases} \rho(X,Y), & \text{if } ac > 0, \\ -\rho(X,Y), & \text{if } ac < 0. \end{cases}$$

For example, the correlation between height and weight of individuals will not be effected by the choice of units of measurement for height (cm, mm, feet) and weight (kg, pounds, grammes) but the covariance (and variance) will change depending upon the choice of units.

Task: Session 7

Attempt the **R Markdown** file for Session 7:
Session 7: Joint distributions

Student Exercises

Attempt the exercises below.

Exercise 13.1.
Show that if X and Y are two independent random variables then $\mathrm{Cov}(X, Y) = 0$.

Exercise 13.2.
Assume that X and Y are two random variables with $\mathrm{Var}(X) = \mathrm{Var}(Y) = \frac{11}{144}$ and $\mathrm{Cov}(X, Y) = -\frac{1}{144}$. Find the variance of $\frac{1}{2}X + Y$.

Chapter 14

Transformations of random variables

14.1 Introduction

In this section we will consider transformations of random variables. Transformations are useful for:

- Simulating random variables.
  For example, computers can generate *pseudo random numbers* which represent draws from $U(0,1)$ distribution and transformations enable us to generate random samples from a wide range of more general (and exciting) probability distributions.

- Understanding functions of random variables.
  Suppose that £P is invested in an account with continuously compounding interest rate r. Then the amount £A in the account after t years is

$$A = P\mathrm{e}^{rt}.$$

  Suppose that $P = 1,000$ and r is a realisation of a continuous random variable R with pdf $f(r)$. What is the p.d.f. of the amount A after one year? *i.e.* What is the p.d.f. of

$$A = 1000\mathrm{e}^{R}?$$

We will consider both univariate and bivariate transformations with the methodology for bivariate transformations extending to more general multivariate transformations.

14.2 Univariate case

Suppose that X is a continuous random variable with p.d.f. $f(x)$. Let g be a continuous function, then $Y = g(X)$ is a continuous random variable. Our aim is to find the p.d.f. of Y.

We present the distribution function method which has two steps:

1. Compute the c.d.f. of Y, that is

$$F_Y(y) = P(Y \leq y).$$

2. Derive the p.d.f. of Y, $f_Y(y)$, using the fact that

$$f_Y(y) = \frac{dF_Y(y)}{dy}.$$

Example 14.2.1. **Square of a Standard Normal**

Let $Z \sim N(0,1)$. Find the p.d.f. of $Y = Z^2$.

For $y > 0$, the c.d.f. of $Y = Z^2$ can be expressed in terms of the c.d.f. of Z,

$$\begin{aligned} F_Y(y) &= P(Y \leq y) \\ &= P(Z^2 \leq y) \\ &= P(-\sqrt{y} \leq Z \leq \sqrt{y}) \\ &= P(Z \leq \sqrt{y}) - P(Z \leq -\sqrt{y}) \\ &= F_Z(\sqrt{y}) - F_Z(-\sqrt{y}). \end{aligned}$$

Note that if we want a specific formula for F_Y, then we can evaluate the resulting c.d.f.'s. In this case:

$$F_Z(\sqrt{y}) = \int_{-\infty}^{\sqrt{y}} \frac{1}{\sqrt{2\pi}} e^{-\frac{z^2}{2}} dz.$$

Therefore, using the chain rule for differentiation,

$$\begin{aligned} f_Y(y) &= \frac{dF_Y(y)}{dy} \\ &= \frac{d}{dy}F_Z(\sqrt{y}) - \frac{d}{dy}F_Z(-\sqrt{y}) \\ &= \frac{d}{dz}F_Z(z)\frac{d}{dy}(z) - \frac{d}{dz}F_Z(-z)\frac{d}{dy}(-z) \end{aligned}$$

where $z = y^{1/2}$.
Now $\frac{d}{dz}F_Z(z) = \frac{1}{\sqrt{2\pi}}e^{-\frac{z^2}{2}}$, so

$$\begin{aligned} f_Y(y) &= \frac{1}{\sqrt{2\pi}}e^{-\frac{(\sqrt{y})^2}{2}}\frac{1}{2\sqrt{y}} - \frac{1}{\sqrt{2\pi}}e^{-\frac{(-\sqrt{y})^2}{2}}\frac{-1}{2\sqrt{y}} \\ &= \frac{1}{2\sqrt{2\pi y}}e^{-\frac{y}{2}} + \frac{1}{2\sqrt{2\pi y}}e^{-\frac{y}{2}} \\ &= \frac{1}{\sqrt{2\pi y}}e^{-\frac{y}{2}}. \end{aligned}$$

Therefore Y has probability density function:

$$f_Y(y) = \begin{cases} \frac{y^{-1/2}}{\sqrt{2\pi}}\exp\left(-\frac{y}{2}\right) & y > 0, \\ 0 & \text{otherwise.} \end{cases}$$

Thus $Y \sim \text{Gamma}\left(\frac{1}{2}, \frac{1}{2}\right)$, otherwise known as a Chi-squared distribution with 1 degree of freedom. :::

14.3 Bivariate case

Suppose that X_1 and X_2 are continuous random variables with joint p.d.f. given by $f_{X_1,X_2}(x_1, x_2)$. Let $(Y_1, Y_2) = T(X_1, X_2)$. We want to find the joint p.d.f. of Y_1 and Y_2.

Definition 14.3.1. **Jacobian**

Suppose $T : (x_1, x_2) \to (y_1, y_2)$ is a one-to-one transformation in some region of $\mathbb{R}^2$, such that $x_1 = H_1(y_1, y_2)$ and $x_2 = H_2(y_1, y_2)$. The *Jacobian* of $T^{-1} = (H_1, H_2)$ is defined by

$$J(y_1, y_2) = \begin{vmatrix} \frac{\partial H_1}{\partial y_1} & \frac{\partial H_1}{\partial y_2} \\ \frac{\partial H_2}{\partial y_1} & \frac{\partial H_2}{\partial y_2} \end{vmatrix}.$$

Theorem 14.3.2. **Transformation of random variables.**

Let $(Y_1, Y_2) = T(X_1, X_2)$ be some transformation of random variables. If T is a one-to-one function and the Jacobian of T^{-1} is non-zero in $T(A)$ where

$$A = \{(x_1, x_2) : f_{X_1,X_2}(X_1, X_2) > 0\},$$

then the joint p.d.f. of Y_1 and Y_2, $f_{Y_1,Y_2}(y_1, y_2)$, is given by

$$f_{X_1,X_2}(H_1(y_1, y_2), H_2(y_1, y_2))|J(y_1, y_2)|$$

if $(y_1, y_2) \in T(A)$, and 0 otherwise.

Example 14.3.3. **Transformation of uniforms.**

Let $X_1 \sim U(0, 1)$, $X_2 \sim U(0, 1)$ and suppose that X_1 and X_2 are independent. Let

$$Y_1 = X_1 + X_2, \quad Y_2 = X_1 - X_2.$$

Find the joint p.d.f. of Y_1 and Y_2.

The joint p.d.f. of X_1 and X_2 is

$$\begin{aligned} f_{X_1,X_2}(x_1, x_2) &= f_{X_1}(x_1) f_{X_2}(x_2) \\ &= \begin{cases} 1, & \text{if } 0 \le x_1 \le 1 \text{ and } 0 \le x_2 \le 1, \\ 0, & \text{otherwise.} \end{cases} \end{aligned}$$

Now $T : (x_1, x_2) \mapsto (y_1, y_2)$ is defined by

$$y_1 = x_1 + x_2, \quad y_2 = x_1 - x_2.$$

Hence,

$$\begin{aligned} x_1 = H_1(y_1, y_2) &= \frac{y_1 + y_2}{2}, \\ x_2 = H_2(y_1, y_2) &= \frac{y_1 - y_2}{2}. \end{aligned}$$

The Jacobian of T^{-1} is

$$J(y_1, y_2) = \begin{vmatrix} \frac{\partial H_1}{\partial y_1} & \frac{\partial H_1}{\partial y_2} \\ \frac{\partial H_2}{\partial y_1} & \frac{\partial H_2}{\partial y_2} \end{vmatrix} = \begin{vmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{vmatrix} = -\frac{1}{2}.$$

Since $A = \{(x_1, x_2) : 0 \leq x_1 \leq 1, 0 \leq x_2 \leq 1\}$ and since the lines $x_1 = 0$, $x_1 = 1$, $x_2 = 0$ and $x_2 = 1$ map to the lines $y_1 + y_2 = 0$, $y_1 + y_2 = 2$, $y_1 - y_2 = 0$ and $y_1 - y_2 = 2$ respectively, it can be checked that

$$T(A) = \{(y_1, y_2) : 0 \leq y_1 + y_2 \leq 2, 0 \leq y_1 - y_2 \leq 2\}.$$

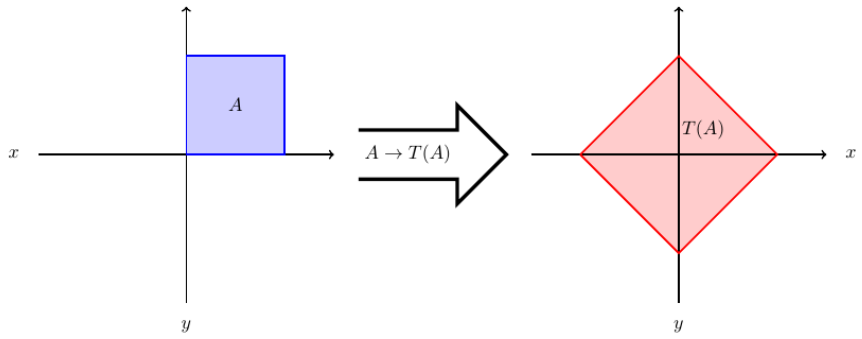


Figure 14.1: Transformation

Thus,

$$f_{Y_1,Y_2}(y_1, y_2) = \begin{cases} \frac{1}{2} f_{X_1,X_2}(H_1(y_1, y_2), H_2(y_1, y_2)), & \text{if } (y_1, y_2) \in T(A), \\ 0, & \text{otherwise.} \end{cases}$$

$$= \begin{cases} \frac{1}{2}, & \text{if } 0 \leq y_1 + y_2 \leq 2 \text{ and } 0 \leq y_1 - y_2 \leq 2, \\ 0, & \text{otherwise.} \end{cases}$$

Example 14.3.4. **Transformation of Exponentials.**

Suppose that X_1 and X_2 are i.i.d. exponential random variables with parameter λ. Let $Y_1 = \frac{X_1}{X_2}$ and $Y_2 = X_1 + X_2$.

(a) Find the joint p.d.f. of Y_1 and Y_2.

(b) Find the p.d.f. of Y_1.

Attempt Example 14.3.4: Transformation of Exponentials and then watch Video 22 for the solutions.

Watch Video 22: Transformation of Exponentials

Solution to Example 14.3.4

Remember from previous results that $Y_2 = X_1 + X_2 \sim \text{Gamma}(2, \lambda)$.

(a) Since X_1 and X_2 are i.i.d. exponential random variables with parameter λ, the joint p.d.f. of X_1 and X_2 is given by

$$\begin{aligned} f_{X_1,X_2}(x_1, x_2) &= f_{X_1}(x_1) f_{X_2}(x_2) \\ &= \begin{cases} \lambda e^{-\lambda x_1} \lambda e^{-\lambda x_2}, & \text{if } x_1, x_2 > 0, \\ 0, & \text{otherwise.} \end{cases} \\ &= \begin{cases} \lambda^2 e^{-\lambda(x_1+x_2)}, & \text{if } x_1, x_2 > 0, \\ 0, & \text{otherwise.} \end{cases} \end{aligned}$$

Solving simultaneously for X_1 and X_2 in terms of Y_1 and Y_2, gives $X_1 = Y_1 X_2$ and

$$Y_2 = X_1 + X_2 = Y_1 X_2 + X_2 = X_2(Y_1 + 1).$$

Rearranging gives $X_2 = \frac{Y_2}{Y_1+1} (= H_2(Y_1, Y_2))$, and then $X_1 = Y_1 X_2 = \frac{Y_1 Y_2}{Y_1+1} (= H_1(Y_1, Y_2))$.
Computing the Jacobian of T^{-1}, we get

$$\begin{aligned} J(y_1, y_2) &= \begin{vmatrix} \frac{\partial H_1}{\partial y_1} & \frac{\partial H_1}{\partial y_2} \\ \frac{\partial H_2}{\partial y_1} & \frac{\partial H_2}{\partial y_2} \end{vmatrix} \\ &= \begin{vmatrix} \frac{y_2}{(y_1+1)^2} & \frac{y_1}{y_1+1} \\ -\frac{y_2}{(y_1+1)^2} & \frac{1}{y_1+1} \end{vmatrix} \\ &= \frac{y_2}{(y_1+1)^3} + \frac{y_1 y_2}{(y_1+1)^3} \\ &= \frac{y_2}{(y_1+1)^2}. \end{aligned}$$

Now,

$$\begin{aligned} A &= \left\{(x_1, x_2) : f_{X_1,X_2}(x_1, x_2) > 0\right\} \\ &= \{(x_1, x_2) : x_1 > 0, x_2 > 0\}. \end{aligned}$$

Therefore, $T(A) \subseteq \{(y_1, y_2) : y_1 > 0, y_2 > 0\}$. Since $x_1 > 0$ and $x_2 > 0$, $y_1 = \frac{x_1}{x_2} > 0$. Furthermore, since $x_1 = \frac{y_1 y_2}{y_1+1} > 0$, then $y_1 y_2 > 0$ implies $y_2 > 0$. Therefore,

$$T(A) = \{(y_1, y_2) : y_1 > 0, y_2 > 0\}.$$

Consequently, the joint p.d.f. of Y_1 and Y_2, $f = f_{Y_1,Y_2}(y_1, y_2)$ is given by

$$\begin{aligned} f &= f_{X_1,X_2}\left(H_1(y_1, y_2), H_2(y_1, y_2)\right) |J(y_1, y_2)| \\ &= f_{X_1,X_2}\left(\frac{y_1 y_2}{1+y_1}, \frac{y_2}{1+y_1}\right) \left|\frac{y_2}{(1+y_1)^2}\right| \\ &= \lambda^2 e^{-\lambda\left(\frac{y_1 y_2}{(1+y_1)} + \frac{y_2}{(1+y_1)}\right)} \frac{y_2}{(1+y_1)^2} \\ &= \lambda^2 e^{-\lambda y_2} \frac{y_2}{(1+y_1)^2}, \quad \text{if } y_1, y_2 > 0. \end{aligned}$$

If either $y_1 < 0$ or $y_2 < 0$, then $f_{Y_1,Y_2}(y_1, y_2) = 0$.

(b) The p.d.f. of Y_1 is the marginal p.d.f. of Y_1 coming from the joint p.d.f $f_{Y_1,Y_2}(y_1, y_2)$. Therefore, for $y_1 > 0$,

$$\begin{aligned} f_{Y_1}(y_1) &= \int_0^\infty \lambda^2 e^{-\lambda y_2} \frac{y_2}{(1+y_1)^2} dy_2 \\ &= \frac{1}{(1+y_1)^2} \int_0^\infty \lambda^2 y_2 e^{-\lambda y_2} dy_2 \\ &= \frac{1}{(1+y_1)^2}. \end{aligned}$$

(In the above integration remember that $\lambda^2 y_2 e^{-\lambda y_2}$ is the p.d.f. of Gamma$(2, \lambda)$.)
So,

$$f_{Y_1}(y_1) = \begin{cases} \frac{1}{(1+y_1)^2} & \text{if } y_1 > 0, \\ 0 & \text{otherwise.} \end{cases}$$

The distribution Y_1 is an example of a probability distribution for which the expectation is not defined.

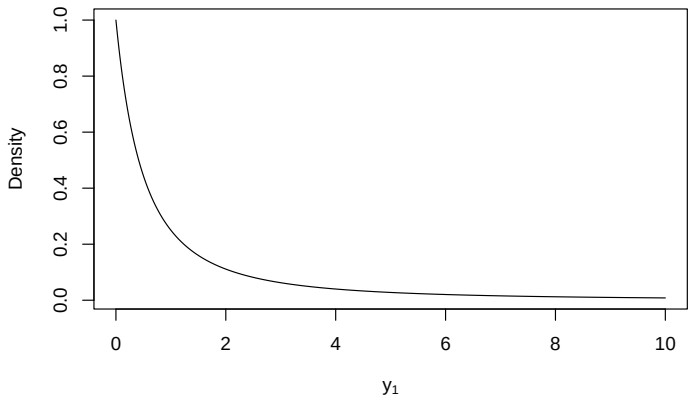


Figure 14.2: Plot of the p.d.f. of Y_1.

Note that one can extend the method of transformations to the case of n random variables.

Student Exercise

Attempt the exercise below.

Exercise 14.1.
Let X and Y be independent random variables, each having probability density function

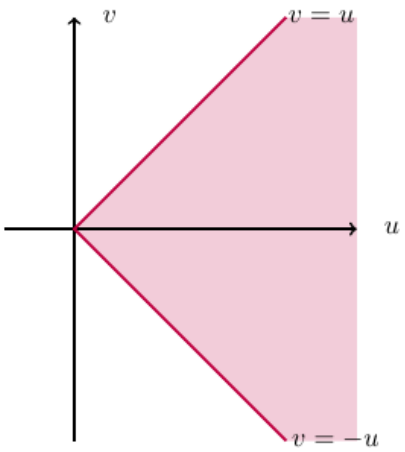
$$f(x) = \begin{cases} \lambda e^{-\lambda x} & \text{if } x > 0, \\ 0 & \text{otherwise} \end{cases}$$

and let $U = X + Y$ and $V = X - Y$.

(a) Find the joint probability density function of U and V.

(b) Hence derive the marginal probability density functions of U and V.

(c) Are U and V independent? Justify your answer.



Chapter 15

Multivariate Normal Distribution

15.1 Introduction

In previous sections we have introduced joint distributions between random variables X and Y and considered their marginal and conditional distributions. In this section, we study the special case where the joint distribution of $X_1, X_2, \ldots, X_n$ is a multivariate normal distribution. In this case both marginal and conditional distributions are (multivariate) normal distributions. We pay particular attention to the special case, $n = 2$, the bivariate normal distribution. Multivariate normal distributions appear in many areas of statistics and being able to manipulate multivariate normal distributions is an important skill.

15.2 n-Dimensional Normal Distribution

Definition 15.2.1. **Multivariate normal distribution**

A random vector $\mathbf{X} = (X_1, X_2, \ldots, X_n)^T$ is said to have an *n-dimensional normal distribution* with parameters $\quad$ and $\quad$ if the joint p.d.f. of $\mathbf{X}$ is given by

$$f_{\mathbf{X}}(\mathbf{x}) = (2\pi)^{-\frac{n}{2}} |\ |^{-\frac{1}{2}} \exp\left\{-\frac{1}{2}(\mathbf{x} - \ )^T \ ^{-1}(\mathbf{x} - \ )\right\},$$

where $\quad = (\mu_1, \mu_2, \ldots, \mu_n)^T$ and $\quad = (\sigma_{ij})$ is an $n \times n$ real, symmetric, positive definite matrix with all positive eigenvalues. It is denoted by

$$\mathbf{X} \sim N_n(\ ,\ ).$$

The multivariate normal distribution has the following important properties:

- If $\mathbf{D}$ is a $p \times n$ matrix and $\mathbf{X} \sim N_n(\ ,\ )$, then $\mathbf{Z} = \mathbf{DX} \sim N_p(\mathbf{D}\ , \mathbf{D}\ \mathbf{D}^T)$.

- The marginal distribution of each component X_i is normal with $E[X_i] = \mu_i$ and $\text{Var}(X_i) = \sigma_{ii}$. Note that this is a direct consequence of the first property taking $\mathbf{D} = (0, \ldots, 0, 1, 0, \ldots, 0)$, that is, the ith component equal to 1.

- The components $X_1, X_2, \ldots, X_n$ of a multivariate normal random vector are independent of each other if and only if $X_1, X_2, \ldots, X_n$ are uncorrelated, i.e. $\sigma_{ij} = \text{Cov}(X_i, X_j) = 0$ for all $i \neq j$.
  That is, for normal random variables uncorrelated (zero covariance) implies independence.

- Conditional distributions derived from joint normal distributions are normal.

Definition 15.2.2. **Bivariate normal distribution**

The *bivariate normal distribution* is the special case $n = 2$ for the n-dimensional normal distribution.

Definition 15.2.3. **Bivariate normal distribution**

The random variables X_1 and X_2 are said to have a *bivariate normal distribution* with mean $= (\mu_1, \mu_2)$ and variance-covariance matrix $= \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$ if their joint p.d.f. is given by

$$f_{X_1,X_2}(x_1, x_2) = \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}} \exp\left\{ -\frac{1}{2(1-\rho^2)} \left[\left(\frac{x_1 - \mu_1}{\sigma_1} \right)^2 \right.\right.$$
$$\left.\left. -2\rho \left(\frac{x_1 - \mu_1}{\sigma_1} \right) \left(\frac{x_2 - \mu_2}{\sigma_2} \right) + \left(\frac{x_2 - \mu_2}{\sigma_2} \right)^2 \right] \right\}.$$

For X_1 and X_2 with a bivariate normal distribution, we have:

- $X_1 \sim N(\mu_1, \sigma_1^2)$ and $X_2 \sim N(\mu_2, \sigma_2^2)$ and $\text{Cov}(X_1, X_2) = \rho\sigma_1\sigma_2$.
- $(X_1 | X_2 = x_2) \sim N\left(\mu_1 + \rho\frac{\sigma_1}{\sigma_2}(x_2 - \mu_2), \sigma_1^2(1-\rho^2)\right)$.
- $(X_2 | X_1 = x_1) \sim N\left(\mu_2 + \rho\frac{\sigma_2}{\sigma_1}(x_1 - \mu_1), \sigma_2^2(1-\rho^2)\right)$.

Suppose that $\mathbf{Z} = (Z_1, Z_2)$, where Z_1 and Z_2 are independent $N(0, 1)$ random variables, that is,

$$\mathbf{Z} \sim N_2(\mathbf{0}, \mathbf{I}_2),$$

where $\mathbf{I}_2$ is the 2×2 identity matrix.

Then for any $\mu = (\mu_1, \mu_2) \in \mathbb{R}^2$ and variance-covariance matrix

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

with $\sigma_1, \sigma_2 > 0$ and $-1 < \rho < 1$,

$$\mathbf{X} \sim N_2(\mu, \Sigma)$$

can be expressed as a transformation of $\mathbf{Z}$. Specifically,

$$\mathbf{X} = \mu + \mathbf{L}\mathbf{Z},$$

where

$$\mathbf{L} = \begin{pmatrix} \sigma_1 & 0 \\ \rho\sigma_2 & \sqrt{1-\rho^2}\sigma_2 \end{pmatrix}.$$

Note that

$$\Sigma = \mathbf{L}\mathbf{L}^\top$$

and this is known as the **Cholesky** decomposition.

The Cholesky decomposition extends to $n \times n$ variance-covariance matrix, Σ and is a common approach to convert n independent univariate normal distributions into a multivariate normal distribution.

Example 15.2.4. **Trivariate normal.**

Suppose $\mathbf{X} = (X_1, X_2, X_3)^T \sim N_3(\mathbf{0}, \ )$, where

$$= \begin{pmatrix} 2 & 1 & 0 \\ 1 & 4 & 0 \\ 0 & 0 & 5 \end{pmatrix}.$$

(a) Find the distribution of $Y = X_1 + X_2$.

(b) Determine the constant c such that $Y_1 = 2X_1 + cX_2$ and $Y_2 = 2X_1 + cX_3$ are independent.

Attempt Example 15.2.4: Trivariate Normal and then watch Video 23 for the solutions.

Watch Video 23: Trivariate Normal

Solution to Example 15.2.4.

(a) Writing $Y = X_1 + X_2$, in the form $\mathbf{DX}$ requires $\mathbf{D} = (1\ 1\ 0)$. By the properties of a multivariate normal distribution

$$Y \sim N(\mathbf{D0}, \mathbf{D}\ \mathbf{D}^T),$$

where $\mathbf{D0} = \mathbf{0}$ and

$$\begin{aligned}\mathbf{D}\,\mathbf{D}^T &= \begin{pmatrix}1 & 1 & 0\end{pmatrix}\begin{pmatrix}2 & 1 & 0\\ 1 & 4 & 0\\ 0 & 0 & 5\end{pmatrix}\begin{pmatrix}1\\ 1\\ 0\end{pmatrix}\\ &= \begin{pmatrix}3 & 5 & 0\end{pmatrix}\begin{pmatrix}1\\ 1\\ 0\end{pmatrix}\\ &= 8.\end{aligned}$$

Therefore, $Y \sim N(0, 8)$.

(b) Let $\mathbf{Y} = \begin{pmatrix}Y_1\\ Y_2\end{pmatrix} = \mathbf{DX}$. Choose

$$\mathbf{D} = \begin{pmatrix}2 & c & 0\\ 2 & 0 & c\end{pmatrix}.$$

By the properties of a multivariate normal distribution, $\mathbf{Y} \sim N_2(\mathbf{D0}, \mathbf{D}\,\mathbf{D}^T)$, where $\mathbf{D0} = \mathbf{0}$ and

$$\begin{aligned}\mathbf{D}\,\mathbf{D}^T &= \begin{pmatrix}2 & c & 0\\ 2 & 0 & c\end{pmatrix}\begin{pmatrix}2 & 1 & 0\\ 1 & 4 & 0\\ 0 & 0 & 5\end{pmatrix}\begin{pmatrix}2 & 2\\ c & 0\\ 0 & c\end{pmatrix}\\ &= \begin{pmatrix}4+c & 2+4c & 0\\ 4 & 2 & 5c\end{pmatrix}\begin{pmatrix}2 & 2\\ c & 0\\ 0 & c\end{pmatrix}\\ &= \begin{pmatrix}8+4c+4c^2 & 8+2c\\ 8+2c & 8+5c^2\end{pmatrix}.\end{aligned}$$

For Y_1 to be independent of Y_2, necessarily $\mathrm{Cov}(Y_1, Y_2) = 8 + 2c = 0$. Therefore $c = -4$.

Task: Session 8

Attempt the **R Markdown** file for Session 8:
Session 8: Transformations and Multivariate Normal Distribution

Chapter 16

Introduction to Linear Models

16.1 Introduction

In this section we present an introduction to Linear Models. Linear Models are the most common type of statistical model and is a wider class of model than is perhaps apparent at first. In Section 16.2, we introduce the concept of constructing a *statistical model*. In Section 16.3 we identify the key (linear) elements for a Linear Model and in Section 16.4 introduce the Normal (Gaussian) linear model. In Section 16.5 we define residuals the differences between the *observations* and what we *expect* to observe given the model. In Section 16.6 we consider *least squares estimation* for the parameters of linear models and show that for the Normal (Gaussian) linear model that this is equivalent to *maximum likelihood estimation*. In Section 16.7 we study two examples and consider how the residuals of the model can help us assess the appropriateness of the model. In Section 16.8 we briefly consider using the linear model for prediction which is one of the main purposes for constructing linear modeals. Finally in Section 16.9 we introduce the concept of nested models where a *simpler* model is *nested* within (a special case of) a *more complex* model. Whether to choose a simple or more complex model is a challenging statistical question and in this section we begin to study some of the considerations needed in making our choice.

16.2 Statistical models

One of the tasks of a statistician is the analysis of data. Statistical analysis usually involves one or more of the following:

- Summarising data;

- Estimation;
- Inference;
- Prediction.

In general, we statistically model the relationship between two or more random variables by considering models of the form:

$$Y = f(\mathbf{X}, \ ) + \epsilon,$$

where,

- Y is the response variable;
- f is some mathematical function;
- $\mathbf{X}$ is some matrix of predictor (input) variables;
- are the model parameters;
- ϵ is the random error term (residual).

If we assume that $E[\epsilon] = 0$, then $E[Y] = f(\mathbf{X}, \ )$ if $\mathbf{X}$ is assumed to be non-random. Otherwise $E[Y|\mathbf{X}] = f(\mathbf{X}, \ )$.

Consider the following examples where such modelling theory could be applied.

Example 16.2.1. **Cars on an intersection**

We observe the number of cars passing an intersection over a one minute interval. We want to estimate the average rate at which cars pass this intersection.

If Y is the number of cars passing the intersection over a one minute interval, then Y is likely to have a Poisson distribution with mean λ. We want to estimate λ, the model parameter.

Example 16.2.2. **Industrial producivity**

In economics, the production of an industry, Y, is modelled to be a function of the amount of labour available, L, and the capital input, K. In particular, the Cobb-Douglas Production Function is given to be $Y = C_0 L^{\alpha} K^{\beta}$.

Furthermore if $\alpha + \beta = 1$, then an industry is said to operate under constant returns to scale, that is, if capital and labour increase by a factor of t, then production also increases by a factor of t.

As a consultant to an economic researcher, you collect production, labour and capital data for a specific industry and want to estimate the functional relationship and test whether $\alpha + \beta = 1$ in this industry. The problem will have the following components:

- A theoretical model: $Y = C_0 L^\alpha K^\beta$;
- A statistical model: $\log Y = C^* + \alpha \log L + \beta \log K + \epsilon$;
- Some estimations: C^*, α and β;
- A test: does $\alpha + \beta = 1$?

Example 16.2.3. **Blood pressure**

Suppose we are interested in studying what factors affect a person's blood pressure. We have a proposed statistical model, where blood pressure depends on a large number of factors:

$$\text{Blood pressure} = f\left(\begin{array}{ccc} \text{age}, & \text{weight}, & \text{gender}, \\ \text{activity level}, & \text{personality type}, & \text{time of day}, \\ & \text{genetic predisposition} & \end{array}\right) + \epsilon.$$

We want to estimate the functional relationship f and potentially test which of the factors has a significant influence on a person's blood pressure.

16.3 The linear model

Suppose that $Y_1, Y_2, \ldots Y_n$ are a collection of response variables, with Y_i dependent on the predictor variables $\mathbf{X}_i = \begin{pmatrix} 1 & X_{1,i} & \cdots & X_{p,i} \end{pmatrix}$. Assume that, for $i = 1, 2, \ldots, n$,

$$Y_i = f(\mathbf{X}_i, \ ) + \epsilon_i = \beta_0 + \beta_1 X_{1i} + \cdots + \beta_p X_{pi} + \epsilon_i.$$

A matrix representation of the model is $\mathbf{Y} = \mathbf{Z} \ + \ $, where

$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix}, \qquad \mathbf{Z} = \begin{bmatrix} 1 & X_{11} & \cdots & X_{p1} \\ 1 & X_{12} & \cdots & X_{p2} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & X_{1n} & \cdots & X_{pn} \end{bmatrix},$$

$$= \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}, \qquad = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}.$$

Here $\mathbf{Z}$ is called the *design matrix* and in models with a constant term includes a column of ones as well as the *data matrix* $\mathbf{X}$ and possibly functions of $\mathbf{X}$. If no constant or functions are included in the model, $\mathbf{Z}$ and $\mathbf{X}$ are equivalent.

It is common to represent linear models in matrix form. As we shall observe in Section 17 using matrices allows for concise representations of key quantities such as parameter estimates and calculating residuals. Familiarity with core concepts from linear algebra is essential in understanding and manipulating linear models.

Definition 16.3.1. **Linear Model**

A model is considered to be *linear* if it is linear in its *parameters*.

Consider the following models, and why they are linear/non-linear:

- $Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \epsilon_i$ is linear;
- $Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i}^2 + \epsilon_i$ is linear;
- $\log Y = \log C_0 L^\alpha K^\beta + \epsilon$ is considered linear since we can transform the model into $\log Y = C_0 + \alpha \log L + \beta \log K + \epsilon$;
- $Y = \frac{\beta_1}{\beta_1 - \beta_2} \left[e^{-\beta_2 X} - e^{\beta_1 X} \right] + \epsilon$ is non-linear.

A linear model therefore has the following underlying assumptions:

- The model form can be written $Y_i = \beta_0 + \beta_1 X_{1i} + \cdots + \beta_p X_{pi} + \epsilon_i$ for all i;
- $E[\epsilon_i] = 0$ for all i;
- $\text{Var}(\epsilon_i) = \sigma^2$ for all i;
- $\text{Cov}(\epsilon_i, \epsilon_j) = 0$ for all $i \neq j$.

16.4 The Normal (Gaussian) linear model

Definition 16.4.1. **Normal Linear Model**

A *normal linear model* assumes:

- A model form given by $Y_i = \beta_0 + \beta_1 X_{1i} + \cdots + \beta_p X_{pi} + \epsilon_i$ for all i;
- $\epsilon_i \sim N(0, \sigma^2)$ are independent and identically distributed (i.i.d.).

There are two key implications of these assumptions:

- $Y_i \sim N(\beta_0 + \beta_1 X_{1i} + \cdots + \beta_p X_{pi}, \sigma^2)$ for all $i = 1, \ldots, n$. Equivalently writing this in matrix form, $\mathbf{Y} \sim N_n(\mathbf{Z}, \sigma^2 \mathbf{I}_n)$ where N_n is the n-dimensional multivariate normal distribution. Note that if two random variables X and Y are normally distributed, then $\text{Cov}(X, Y) = 0$ if and only if X and Y are independent.
- Since $\text{Cov}(\epsilon_i, \epsilon_j) = 0$ for all $i \neq j$, then $\text{Cov}(Y_i, Y_j) = 0$ for all $i \neq j$, and $Y_1, Y_2, \ldots, Y_n$ are independent. (Remember that for Normal (Gaussian) random variables X and Y are independent if and only if they are uncorrelated $Cov(X, Y) = 0$, see Section 15.2.)

16.5 Residuals

We have the statistical model:

$$Y = f(\mathbf{X}, \beta) + \epsilon,$$

which satisfies $E[\epsilon] = 0$, and hence, $E[Y] = f(\mathbf{X}, \beta)$. The above equation can be rewritten as

$$\epsilon = Y - f(\mathbf{X}, \beta).$$

Suppose that we have **observed** responses $y_1, y_2, \ldots, y_n$, where observation i has predictors $\mathbf{x}_i$. Then given parameters β, the **expected** value for the i^{th} response is $f(\mathbf{x}_i, \beta)$, and is often denoted $\widehat{y}_i$. The residual ϵ_i is the difference between the observed response and its expected value:

$$\epsilon_i = y_i - \widehat{y}_i = y_i - f(\mathbf{x}_i, \beta).$$

Note that if $f(\mathbf{x}_i, \beta) = \alpha + \beta x_i$, then

$$\epsilon_i = y_i - \{\alpha + \beta x_i\}.$$

An assumption of the Normal linear model is that $\epsilon_i \sim N(0, \sigma^2)$, independent of the value of $f(x_i, \beta) = \alpha + \beta x_i$. Therefore plotting residual values against expected values is one way of testing the appropriateness of the model.

16.6 Straight Line, Horizontal Line and Quadratic Models

In this section we look at three types of linear model that we might choose to assume to fit some data X_i and Y_i. Making this choice appropriately is a key part of the statistical analysis process.

Definition 16.6.1. **Straight line model**

The **straight line model** is the simple linear regression model given by

$$y_i = \alpha + \beta x_i + \epsilon_i, \qquad \text{for all } i = 1, \ldots n.$$

Given a straight line model, we have $E[Y] = \alpha + \beta X$. The key part of using a straight line model is to estimate the values of α and β.

Definition 16.6.2.
Let $\hat{\alpha}$ and $\hat{\beta}$ be the estimated values of α and β, respectively. We call y_i the i^{th} *observed value* and $\hat{y}_i = \hat{\alpha} + \hat{\beta} x_i$ the i^{th} *fitted value* (expected value).

Definition 16.6.3. **Model deviance**

$D = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$ is called the *model deviance*.

Since $\epsilon_i = y_i - \hat{y}_i$, the model deviance is the sum of the squares of the residuals,

$$D = \sum_{i=1}^{n} \epsilon_i^2.$$

For the estimated line to fit the data well, one wants an estimator of α and β that minimises the model deviance. So, choose $\hat{\alpha}$ and $\hat{\beta}$ to minimise

$$D = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y_i - \alpha - \beta x_i)^2 .$$

To minimise D we calculate the stationary points of D, that is, the values of α and β for which the two first order partial derivatives vanish.

$$\frac{\partial D}{\partial \alpha} = -2\sum_{i=1}^{n}\left(y_i - \left(\hat{\alpha} + \hat{\beta}x_i\right)\right) = 0$$

$$\frac{\partial D}{\partial \beta} = -2\sum_{i=1}^{n} x_i\left(y_i - \left(\hat{\alpha} + \hat{\beta}x_i\right)\right) = 0$$

Solving these equations simultaneously gives

$$\hat{\beta} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} = \frac{(n-1)s_{xy}}{(n-1)s_x^2} = \frac{s_{xy}}{s_x^2},$$

$$\hat{\alpha} = \bar{y} - \hat{\beta}\bar{x}.$$

Note that $\hat{\alpha}$ and $\hat{\beta}$ are called *least squares estimators* of α and β. We did not use the normality assumption in our derivation, so the least squares estimators are invariant to the choice of distribution for the error terms.

If we include the assumption of normality, then it can be shown that $\hat{\alpha}$ and $\hat{\beta}$ are also the MLEs of α and β respectively.

Lemma 16.6.4.
Let $y_1, y_2, \ldots, y_n$ be observations from a normal linear model:

$$y = \alpha + \beta x + \epsilon,$$

where $\epsilon \sim N(0, \sigma^2)$ and $x_1, x_2, \ldots, x_n$ are the predictor variables. Then

$$\hat{\beta} = \frac{s_{xy}}{s_x^2} \qquad \text{and} \qquad \hat{\alpha} = \bar{y} - \hat{\beta}\bar{x},$$

are the maximum likelihood estimates of β and α, respectively.

First, note that

$$y_i \sim N(\alpha + \beta x_i, \sigma^2).$$

Therefore the likelihood is given by

$$\begin{aligned} L(\alpha, \beta, \sigma^2) &= \prod_{i=1}^{n} f(y_i|\alpha, \beta, x_i, \sigma^2) \\ &= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}\left\{y_i - (\alpha + \beta x_i)\right\}^2\right) \\ &= (2\pi\sigma^2)^{-\frac{n}{2}} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n}\left\{y_i - (\alpha + \beta x_i)\right\}^2\right). \end{aligned}$$

The log-likelihood is

$$l(\alpha, \beta, \sigma^2) = -\frac{n}{2}\log\left(2\pi\sigma^2\right) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}\left\{y_i - (\alpha + \beta x_i)\right\}^2.$$

In order to maximise the log-likelihood with respect to α and β, we note that:

- $-\frac{n}{2}\log\left(2\pi\sigma^2\right)$ does not involve α and β, so can be treated as a constant;
- Since $\sigma^2 > 0$, $-\frac{1}{2\sigma^2}\sum_{i=1}^{n}\left\{y_i - (\alpha + \beta x_i)\right\}^2$ will reach its maximum when $\sum_{i=1}^{n}\left\{y_i - (\alpha + \beta x_i)\right\}^2$ is minimised.

Therefore the parameter values $\hat{\alpha}$ and $\hat{\beta}$ which maximise $l(\alpha, \beta, \sigma^2)$ are the parameter values which minimise $\sum_{i=1}^{n}\left\{y_i - (\alpha + \beta x_i)\right\}^2$, *i.e.* the *least squares estimates*.

Note that the maximum likelihood estimates of $\hat{\alpha}$ and $\hat{\beta}$ do not depend on the value of σ^2.

Definition 16.6.5. **Horizontal line model**

The **horizontal line model** is the simple linear regression model given by

$$y_i = \mu + \epsilon_i, \qquad \text{for } i = 1, \ldots, n.$$

Given a horizontal line model, we have $E[Y] = \mu$. Specifically in this model, we assume the predictor variable has no ability to explain the variance in the response variable.

To estimate μ by least squares we minimise $D = \sum_{i=1}^{n}(y_i - \mu)^2$. Setting $\frac{\partial D}{\partial \mu} = 0$ and solving, we get $\hat{\mu} = \bar{y}$.

Let D_1 be the deviance of the straight line model and D_2 be the deviance of the horizontal line model. The straight line model does a better job of explaining the variance in Y if $D_1 \leq D_2$, in which case we say that the straight line model *fits* the data better.

Definition 16.6.6. **Quadratic line model**

The **quadratic model** is the simple linear regression model given by

$$y_i = \alpha + \beta x_i + \gamma x_i^2 + \epsilon_i, \qquad \text{for } i = 1, \ldots, n.$$

To estimate α, β and γ by least squares we minimise

$$D = \sum_{i=1}^{n} \left(y_i - (\alpha + \beta x_i + \gamma x_i^2)\right)^2.$$

If we let $D_3 = \sum_{i=1}^{n} \left(y_i - (\hat{\alpha} + \hat{\beta} x_i + \hat{\gamma} x_i^2)\right)^2$ be the model deviance, then the quadratic model *fits* the data better than the straight line model if $D_3 \leq D_1$.

16.7 Examples

Example 16.7.1. **Tyre experiment**

A laboratory tests tyres for tread wear by conducting an experiment where tyres from a particular manufacturer are mounted on a car. The tyres are rotated from wheel to wheel every 1000 miles, and the groove depth is measured in mils (0.001 inches) initially and after every 4000 miles giving the following data (Tamhane and Dunlap, 2000):

Mileage (1000 miles)	Groove Depth (mils)
0	394.23
4	329.50
8	291.00
12	255.17
16	229.33
20	204.83
24	179.00
28	163.83
32	150.33

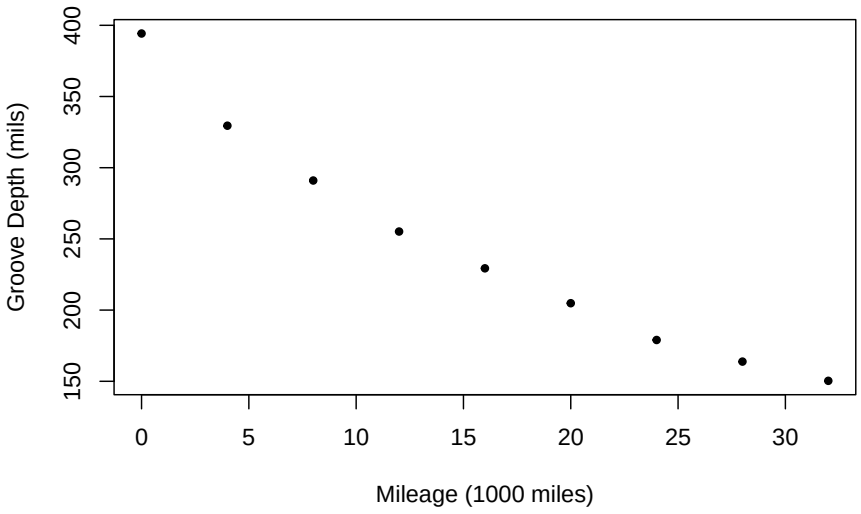
Watch Video 24 for a work through fitting linear models to the tyre experiment

in **R** and a discussion of choosing the most appropriate linear model. A work through of the analysis is presented below.

Watch Video 24: Tyre Experiment

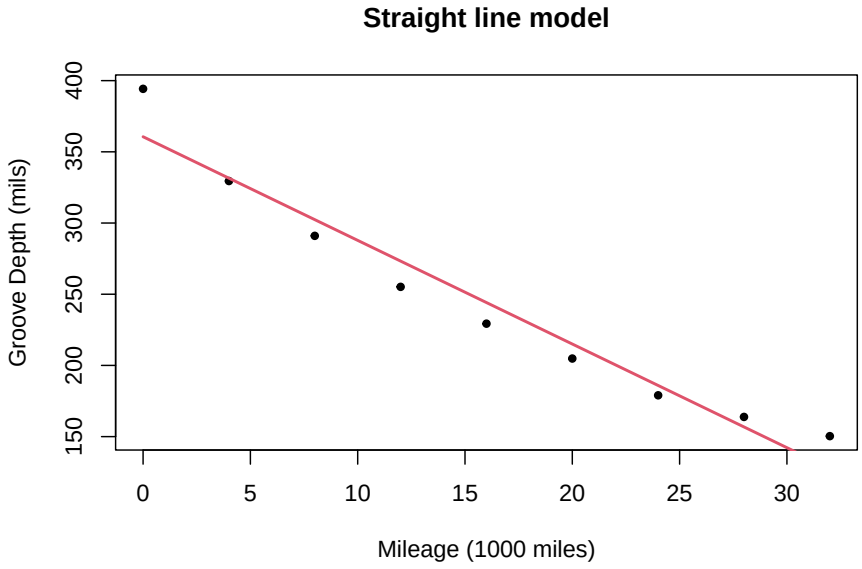
Firstly we have to determine which is the response variable and which is the predictor (or controlled) variable. Secondly, we have to hypothesise a functional relationship between the two variables, using either theoretical relationships or exploratory data analysis.

Let the response variable, Y, be groove depth and let the predictor variable, X, be mileage. Consider a plot of mileage vs. depth:



Note that as mileage increases, the groove depth decreases.

The straight line model for the data is

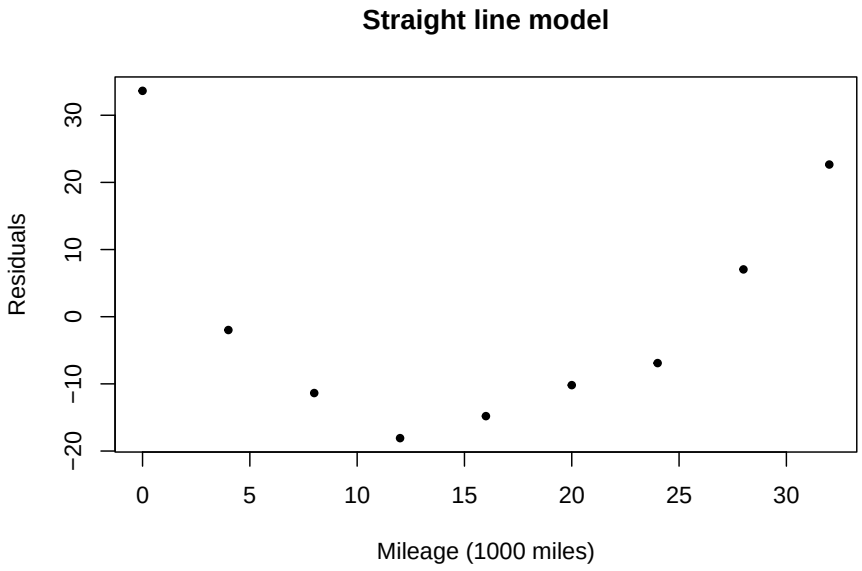


The straight line model is:

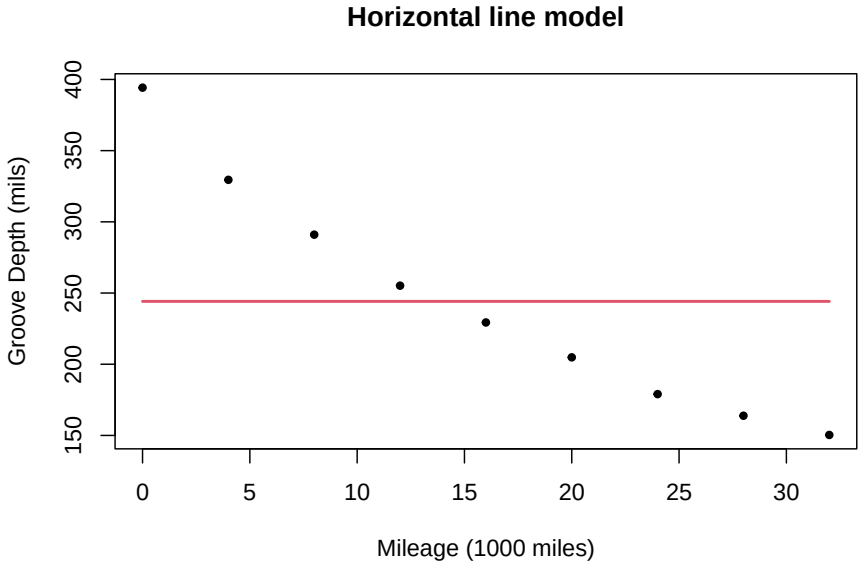
$$y = 360.599 - 7.279x + \epsilon$$

and the deviance for the model is 2524.8.

A plot of the residuals for the straight line model shows a relationship with x (mileage), possibly quadratic. This informs us that there is a relationship between mileage and groove depth which is not captured by the linear model.



The horizontal line model for the data is

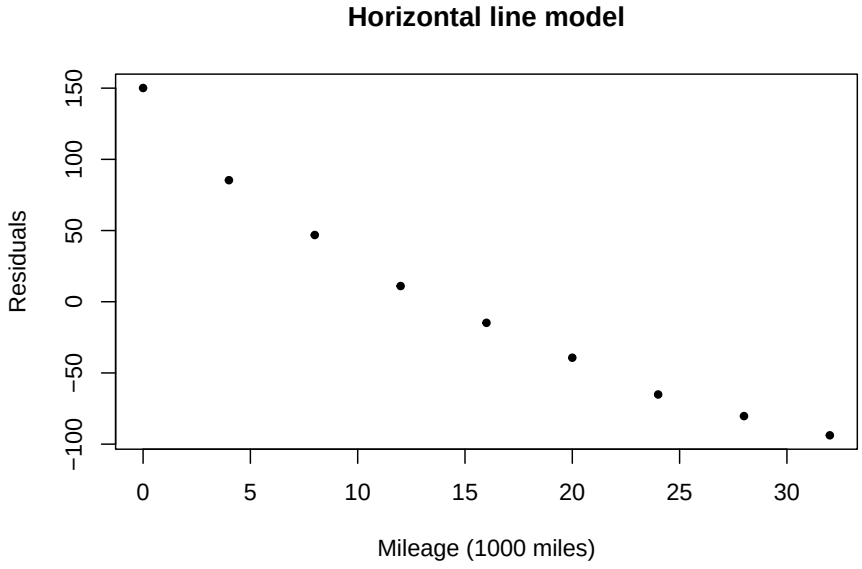


The horizontal line model is:

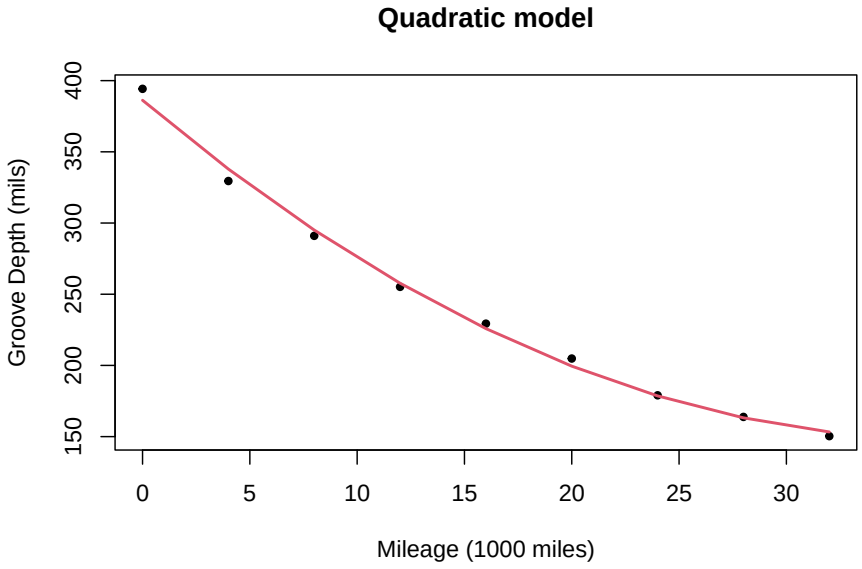
$$y = 244.136 + \epsilon.$$

The deviance for the model is 53388.7, which is much higher than the deviance for the straight line model suggesting it is a considerably worse fit to the data. In this case the poorness of the fit of the horizontal line model is obvious, but later will explore ways of making rigorous the comparison between models.

A plot of the residuals for the horizontal line model shows a very clear downward trend with x (mileage) confirming that the horizontal line model does not capture the relationship between mileage and groove depth.



The quadratic model for the data is

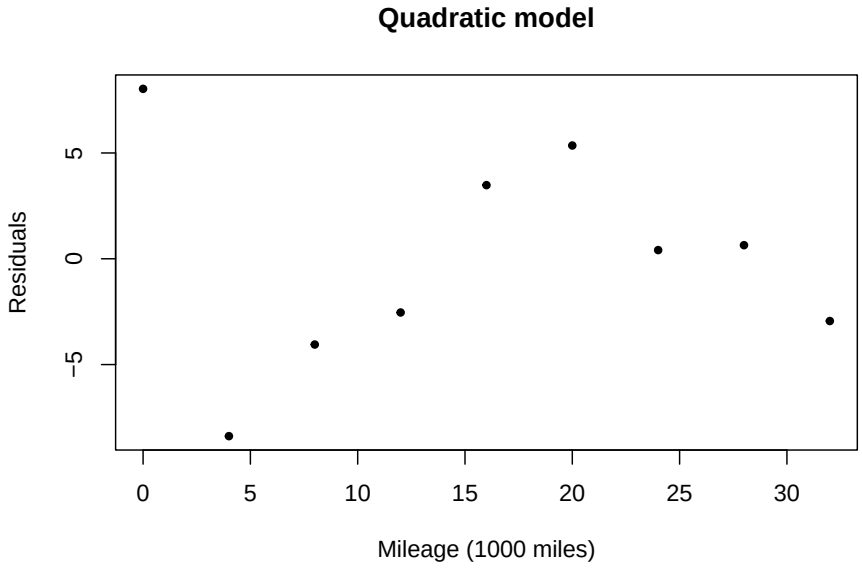


The quadratic model is

$$y = 386.199 - 12.765x + 0.171x^2 + \epsilon$$

and the deviance for the model is 207.65. This is a substantial reduction on the deviance of the straight line model suggesting that it offers a substantial improvement.

A plot of the residuals for the quadratic model shows no obvious pattern. This suggests that the model could be appropriate in capturing the relationship between mileage and groove depth, with the differences between *observed* and *expected* values due to randomness.



Example 16.7.2. **Drug effectiveness**

Suppose we are interested in the effect a certain drug has on the weight of an organ. An experiment is designed in which rats are randomly assigned to different treatment groups in which each group contains J rats and receives the drug at one of 7 distinct levels. Upon completion of the treatment, the organs are harvested from the rats and weighed.

Let Y_{ij} be the weight of the organ (response variable) of the j^{th} rat in the i^{th} treatment,

$$Y_{ij} = \mu_i + \epsilon_{ij}, \qquad \text{for all } i = 1, \dots, 7 \text{ and } j = 1, \dots, J.$$

The model is linear in the parameters $\mu_1, \mu_2, \dots, \mu_7$. Specifically our aim is to test whether $\mu_1 = \mu_2 = \cdots = \mu_7$. Estimating using least squares minimises

$$D = \sum_{i=1}^{7} \sum_{j=1}^{J} (y_{ij} - \mu_i)^2,$$

and least squares estimators are given by:

$$\hat{\mu}_i = \bar{y}_{i\cdot} = \frac{1}{J} \sum_{i=1}^{J} y_{ij}.$$

The estimate of the mean for level i is the sample mean of the J rats receiving treatment level i.

16.8 Prediction

A linear model identifies a relationship between the response variable y and the predictor variable(s), $\mathbf{x}$. We can then use the linear model to predict y^* given predictor variables $\mathbf{x}^*$.

Given the model,

$$Y = f(\mathbf{x}, \beta) + \epsilon$$

where $E[\epsilon] = 0$, we have that our best estimate of y^* given $\mathbf{x}^*$ and model parameters $\hat{\beta}$ is

$$y^* = E[Y|\mathbf{x}^*, \hat{\beta}] = f(\mathbf{x}^*, \hat{\beta}) = \hat{\beta}_0 + \sum_{j=1}^{p} \hat{\beta}_j x_j^*.$$

We will discuss later the uncertainty in the prediction of y^* which depends upon the variance of ϵ, uncertainty in the estimation of $\hat{\beta}$ and how far the x_j^*s are from the mean of the x_js.

For Example 16.7.1 (Tyre experiment), we can use the three models (straight line, horizontal line, quadratic) to predict the groove depth (mils) of the tyres after 18,000 miles. The predicted values are:

- Straight line model - $y^* = 360.599 - 7.279(18) = 229.577$.
- Horizontal line model - $y^* = 244.136$.
- Quadratic model - $y^* = 386.199 - 12.765(18) + 0.171(18^2) = 211.833$.

16.9 Nested Models

In Example 16.7.1 (Tyre experiment), we considered three models:

- Straight line model: $y = \alpha + \beta x + \epsilon$.
- Horizontal line model: $y = \mu + \epsilon$.
- Quadratic model: $y = \alpha + \beta x + \gamma x^2 + \epsilon$.

The quadratic model is the most general of the three models. We note that if $\gamma = 0$, then the quadratic model reduces to the straight line model. Similarly letting $\beta = \gamma = 0$ in the quadratic model and with $\mu = \alpha$, the quadratic model reduces to the horizontal model. That is, the horizontal line and straight line models are special cases of the quadratic model, and we say that the horizontal line and straight line models are **nested models** in the quadratic model. Similarly the horizontal line model is a **nested model** in the straight line model.

Definition 16.9.1. **Nested model**

Model A is a nested model of Model B if the parameters of Model A are a subset of the parameters of Model B.

Lemma 16.9.2.
Let D_A and D_B denote the deviances of Models A and B, respectively. Then if Model A is a nested model of Model B,

$$D_B \leq D_A.$$

That is, the more complex model with additional parameters will fit the data better.

Let $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_K)$ denote the K parameters of Model A and let $\beta = (\alpha_1, \alpha_2, \ldots, \alpha_K, \delta_1, \ldots, \delta_M)$ denote the $K + M$ parameters of Model B.

If $\hat{\alpha} = (\hat{\alpha}_1, \hat{\alpha}_2, \ldots, \hat{\alpha}_K)$ minimise the deviance under Model A, then the parameters $(\hat{\alpha}_1, \hat{\alpha}_2, \ldots, \hat{\alpha}_K, 0, \ldots, 0)$, where $\delta_i = 0$ will achieve the deviance D_A under Model B. Thus D_B can be at most equal to D_A.

Since more complex models will better fit data (smaller deviance), why not choose the most complex model possible?

There are many reasons and these include *interpretability*, can you interpret the relation between x_i and y_i (for example, the time taken to run 100 metres is unlikely to be a good predictor for performance on a maths test) and *predictive power*, given a new predictor observation x^* can we predict y^*.

Student Exercise

Attempt the exercise below.

Exercise 16.1.
Given the following theoretical relationships between Y and X, with α and β unknown, can you find ways of expressing the relationship in a **linear** manner?

(a) $Y = \alpha e^{\beta X}$,

(b) $Y = \alpha X^{\beta}$,

(c) $Y = \log(\alpha + e^{\beta X})$.

Chapter 17

Least Squares Estimation for Linear Models

17.1 Introduction

In Section 16 we introduced linear models with particular emphasis on Normal linear models. We derived the *least square estimates* of the model parameters for the straight line model:

$$y = \alpha + \beta x + \epsilon,$$

and showed that if $\epsilon \sim N(0, \sigma^2)$ then the least square estimates coincide with the *maximum likelihood estimates* of the parameters. In this section we consider the mathematics behind least squares estimation for general linear models. This relies heavily on linear algebra (matrix manipulation) and we give a review of key linear algebra results in Section 17.2. The main message is that we can concisely express key quantities such as least square parameter estimates, $\widehat{\beta}$, fitted values, $\widehat{y}$ and residuals, ϵ as functions of matrices.

17.2 Linear algebra review

Definition 17.2.1. **Rank of a matrix**
Let $\mathbf{M}$ be any $n \times m$ matrix. Then the *rank* of $\mathbf{M}$ is the maximum number of linearly independent column vectors of $\mathbf{M}$.

Definition 17.2.2. **Transpose of a matrix**
If $\mathbf{M} = (m_{ij})$, then $\mathbf{M}^T = (m_{ji})$ is said to be the *transpose* of the matrix $\mathbf{M}$.

Definition 17.2.3. **Properties of square matrices**
Suppose $\mathbf{A}$ is a square $n \times n$ matrix, then

- $\mathbf{A}$ is *symmetric* if and only if $\mathbf{A}^T = \mathbf{A}$;
- $\mathbf{A}^{-1}$ is the *inverse* of $\mathbf{A}$ if and only if $\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}_n$;
- The matrix $\mathbf{A}$ is *nonsingular* if and only if $\text{rank}(\mathbf{A}) = n$;
- $\mathbf{A}$ is *orthogonal* if and only if $\mathbf{A}^{-1} = \mathbf{A}^T$;
- $\mathbf{A}$ is *idempotent* if and only if $\mathbf{A}^2 = \mathbf{A}\mathbf{A} = \mathbf{A}$;
- $\mathbf{A}$ is *positive definite* if and only if $\mathbf{x}^T\mathbf{A}\mathbf{x} > 0$ for all non-zero vectors $\mathbf{x}$.

Note the following two important results:

- $\mathbf{A}$ has an inverse if and only if $\mathbf{A}$ is nonsingular, that is the rows and columns are linearly independent;
- $\mathbf{A}^T\mathbf{A}$ is positive definite if $\mathbf{A}$ has an inverse.

The following computational results are also useful:

- Let $\mathbf{N}$ be an $n \times p$ matrix and $\mathbf{P}$ be a $p \times n$ matrix, then

$$(\mathbf{N}\mathbf{P})^T = \mathbf{P}^T\mathbf{N}^T;$$

- Suppose $\mathbf{A}$ and $\mathbf{B}$ are two invertible $n \times n$ matrices, then

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

- We can write the sum of squares $\sum_{i=1}^{n} x_i^2 = \mathbf{x}^T\mathbf{x}$, where $\mathbf{x}^T = [x_1, x_2, \ldots, x_n]$ is a $1 \times n$ row vector.

Given n-dimensional vectors $\mathbf{x}$ and $\mathbf{y} = \mathbf{y}(\mathbf{x})$, we define

$$\frac{d\mathbf{y}}{d\mathbf{x}} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_n}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_n}{\partial x_2} \\ \vdots & \vdots & \vdots \\ \frac{\partial y_1}{\partial x_n} & \cdots & \frac{\partial y_n}{\partial x_n} \end{pmatrix}.$$

Then the following results hold in the calculus of matrices:

- $\frac{d}{d\mathbf{x}}(\mathbf{A}\mathbf{x}) = \mathbf{A}^T$, where $\mathbf{A}$ is a matrix of constants;
- $\frac{d}{d\mathbf{x}}(\mathbf{x}^T\mathbf{A}\mathbf{x}) = (\mathbf{A} + \mathbf{A}^T)\mathbf{x} = 2\mathbf{A}\mathbf{x}$ whenever $\mathbf{A}$ is symmetric;

- If $f(\mathbf{x})$ is a function of several variables the necessary condition to maximise or minimise $f(\mathbf{x})$ is

$$\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} = 0.$$

- Let $\mathbf{H} = \frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^T}$ be the Hessian of f, that is the matrix of second derivatives. Then a maximum will occur if $\mathbf{H}$ is negative definite, and a minimum will occur if $\mathbf{H}$ is positive definite.

Let $\mathbf{A}$ be a matrix of constants and $\mathbf{Y}$ be a random vector, then we have the following expectation and variance results:

- $E[\mathbf{AY}] = \mathbf{A}E[\mathbf{Y}]$;
- $\text{Var}(\mathbf{AY}) = \mathbf{A}\text{Var}(\mathbf{Y})\mathbf{A}^T$.

17.3 Deriving the least squares estimator

Recall that a linear model is given in matrix form by $\mathbf{Y} = \mathbf{Z} + \ $, where

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}, \qquad \mathbf{Z} = \begin{pmatrix} 1 & X_{11} & \cdots & X_{(p-1)1} \\ 1 & X_{12} & \cdots & X_{(p-1)2} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & X_{1n} & \cdots & X_{(p-1)n} \end{pmatrix},$$

$$= \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p-1} \end{pmatrix}, \qquad = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix},$$

where

- $\mathbf{Y}$ is an $n \times 1$ column vector of observations of the response variable;
- $\mathbf{Z}$ is the $n \times p$ design matrix whose first column is a column of 1's, if there is a constant in the model. The other columns are the observations on the explanatory variables $(X_1, X_2, \ldots, X_{p-1})$;
- is a $p \times 1$ column vector of the unknown parameters;
- is an $n \times 1$ column vector of the random error terms.

The general linear regression model assumes that $E[\ ] = \mathbf{0}$ and $\text{Var}(\ ) = \sigma^2 \mathbf{I}_n$.

Our aim is to estimate the unknown vector of parameters, .

Theorem 17.3.1. **Least squares estimate**
The least squares estimate of is

$$\hat{} = (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{y}.$$

The least squares estimator is the value of that minimises the model deviance D. Consider

$$\begin{aligned} D &= \sum_{i=1}^{n}(\mathbf{y}_i - (\mathbf{Z}\ )_i)^2 \\ &= (\mathbf{y} - \mathbf{Z}\ )^T(\mathbf{y} - \mathbf{Z}\ ) \\ &= \mathbf{y}^T\mathbf{y} - \mathbf{y}^T\mathbf{Z}\ -\ {}^T\mathbf{Z}^T\mathbf{y} +\ {}^T\mathbf{Z}^T\mathbf{Z} \\ &= \mathbf{y}^T\mathbf{y} - 2\mathbf{y}^T\mathbf{Z}\ +\ {}^T\mathbf{Z}^T\mathbf{Z}\ . \end{aligned}$$

Taking the derivative of D with respect to and noticing that $\mathbf{Z}^T\mathbf{Z}$ is a symmetric matrix, we have that

$$\begin{aligned} \frac{\partial D}{\partial} &= (-2\mathbf{y}^T\mathbf{Z})^T + 2\mathbf{Z}^T\mathbf{Z} \\ &= -2\mathbf{Z}^T\mathbf{y} + 2\mathbf{Z}^T\mathbf{Z}\ . \end{aligned}$$

Therefore the least squares estimator$\hat{}$ of will satisfy $\mathbf{Z}^T\mathbf{Z}\ = \mathbf{Z}^T\mathbf{y}$. This system of equations are the *normal equations* for the general linear regression model. To be able to isolate$\hat{}$ it is necessary for $\mathbf{Z}^T\mathbf{Z}$ to be invertible. Therefore we need $\mathbf{Z}$ to be of full rank, that is, rank$(\mathbf{Z}) = p$. If rank$(\mathbf{Z}) = p$, then

$$\hat{} = (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{y}.$$

We know that$\hat{}$ minimising D is equivalent to the Hessian of D will be positive definite. If $\mathbf{Z}$ has full rank, then since $\mathbf{Z}^T\mathbf{Z}$ is a symmetric matrix, we have that

$$\begin{aligned} \mathbf{H} &= \frac{\partial^2 D}{\partial\ ^2} \\ &= (2\mathbf{Z}^T\mathbf{Z})^T \\ &= 2\mathbf{Z}^T\mathbf{Z}. \end{aligned}$$

We know $\mathbf{Z}^T\mathbf{Z}$ is positive definite and hence,$\hat{}$ is the least squares estimator of .

Let $\hat{\mathbf{y}} = \mathbf{Z}$ be the $n \times 1$ vector of *fitted values* of $\mathbf{y}$. Note that

$$\hat{\mathbf{y}} = \mathbf{Z} = \mathbf{Z}(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{y}.$$

If we set $\mathbf{P} = \mathbf{Z}(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T$, then we can write

$$\hat{\mathbf{y}} = \mathbf{P}\mathbf{y}.$$

The matrix $\mathbf{P}$ is therefore often referred to as the *hat matrix*. Note that P is symmetric and idempotent because $\mathbf{P}^T = \mathbf{P}$ and $\mathbf{P}^2 = \mathbf{P}$.

The residuals, ϵ, satisfy

$$\epsilon = \mathbf{y} - \hat{\mathbf{y}} = \mathbf{I}_n\mathbf{y} - \mathbf{P}\mathbf{y} = (\mathbf{I}_n - \mathbf{P})\mathbf{y},$$

where $\mathbf{I}_n$ is the $n \times n$ identify matrix.

Therefore the sum of the square of the residuals is given by

$$\begin{aligned}\sum_{i=1}^{n} \epsilon_i^2 &= (\mathbf{y} - \mathbf{Z})^T(\mathbf{y} - \mathbf{Z}) \\ &= ((\mathbf{I}_n - \mathbf{P})\mathbf{y})^T(\mathbf{I}_n - \mathbf{P})\mathbf{y} \\ &= \mathbf{y}^T(\mathbf{I}_n - \mathbf{P})^T(\mathbf{I}_n - \mathbf{P})\mathbf{y}.\end{aligned}$$

Theorem 17.3.2.
The quantity

$$s^2 = \frac{1}{n-p}\sum_{i=1}^{n} \epsilon_i^2 = \frac{1}{n-p}(\mathbf{y} - \mathbf{Z})^T(\mathbf{y} - \mathbf{Z})$$

is an unbiased estimator of σ^2.

Note that to obtain an unbiased estimator of σ^2, we divide the sum of the square of the residuals by $n-p$. That is, the **number of observations** (n) minus the **number of parameters** (p) estimated in β. This is in line with the divisor $n-1$ in estimating the variance of a random variable X from data $x_1, x_2, \ldots, x_n$ with $\mu = E[X]$ (one parameter) estimated by $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$.

17.4 Examples

Example 17.4.1.
Suppose we have two observations such that

$$y_1 = \theta + \epsilon,$$
$$y_2 = 2\theta + \epsilon.$$

Calculate the least squares estimator of θ.

Writing the given linear model in a matrix format, one obtains

$$\mathbf{Z} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \qquad \text{and} \qquad \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

Then $(\mathbf{Z}^T\mathbf{Z})^{-1} = \frac{1}{5}$ and by applying Theorem 17.3.1 (Least squares estimate):

$$\hat{\theta} = (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{Y} = \frac{1}{5}(y_1 + 2y_2).$$

Example 17.4.2. **Simple Linear Regression**
Consider the simple regression model, $y_i = a + bx_i + \epsilon$, for $i \in \{1, \dots, n\}$. Then in matrix terms $\mathbf{Y} = \mathbf{Z}\ +\ $ where,

$$\mathbf{Y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}, \qquad \mathbf{Z} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix},$$

$$= \begin{pmatrix} a \\ b \end{pmatrix}, \qquad = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}.$$

Calculate the least squares estimator of .

The least squares estimators of will be given by,

$$\hat{} = (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{y},$$

where,

$$\mathbf{Z}^T\mathbf{Z} = \begin{pmatrix} 1 & 1 & \cdots 1 \\ x_1 & x_2 & \cdots x_n \end{pmatrix} \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}$$

$$= \begin{pmatrix} n & \sum_{i=1}^{n} x_i \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 \end{pmatrix},$$

$$\mathbf{Z}^T\mathbf{y} = \begin{pmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i y_i \end{pmatrix}.$$

Therefore, the inverse of $\mathbf{Z}^T\mathbf{Z}$ is

$$(\mathbf{Z}^T\mathbf{Z})^{-1} = \frac{1}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \begin{pmatrix} \frac{1}{n}\sum_{i=1}^{n} x_i^2 & -\bar{x} \\ -\bar{x} & 1 \end{pmatrix},$$

and so

$$
\begin{aligned}
\hat{} &= \left(\mathbf{Z}^T\mathbf{Z}\right)^{-1}\mathbf{Z}^T\mathbf{y} \\
&= \frac{1}{\sum_{i=1}^{n}(x_i-\bar{x})^2}\begin{pmatrix} \frac{1}{n}\sum_{i=1}^{n}x_i^2 & -\bar{x} \\ -\bar{x} & 1 \end{pmatrix}\begin{pmatrix} \sum_{i=1}^{n}y_i \\ \sum_{i=1}^{n}x_iy_i \end{pmatrix} \\
&= \frac{1}{\sum_{i=1}^{n}(x_i-\bar{x})^2}\begin{pmatrix} \frac{1}{n}\sum_{i=1}^{n}x_i^2\sum_{i=1}^{n}y_i - \bar{x}\sum_{i=1}^{n}x_iy_i \\ -\bar{x}\sum_{i=1}^{n}y_i + \sum_{i=1}^{n}x_iy_i \end{pmatrix} \\
&= \frac{1}{\sum_{i=1}^{n}(x_i-\bar{x})^2}\begin{pmatrix} \bar{y}\sum_{i=1}^{n}x_i^2 - \bar{x}\sum_{i=1}^{n}x_iy_i \\ \sum_{i=1}^{n}y_i(x_i-\bar{x}) \end{pmatrix} \\
&= \frac{1}{\sum_{i=1}^{n}(x_i-\bar{x})^2}\begin{pmatrix} \bar{y}\sum_{i=1}^{n}(x_i-\bar{x})^2 - \bar{x}\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y}) \\ \sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y}) \end{pmatrix} \\
&= \begin{pmatrix} \bar{y} - \bar{x}\frac{\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y})}{\sum_{i=1}^{n}(x_i-\bar{x})^2} \\ \frac{\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y})}{\sum_{i=1}^{n}(x_i-\bar{x})^2} \end{pmatrix}.
\end{aligned}
$$

So,

$$
\begin{pmatrix} \hat{a} \\ \hat{b} \end{pmatrix} = \begin{pmatrix} \bar{y} - \hat{b}\bar{x} \\ \frac{s_{xy}}{s_x^2} \end{pmatrix}.
$$

The least square estimates agree with the estimates we obtained in Section 16.6.

17.5 Properties of the estimator of

In this section we give a collection of results about the properties of the estimator of . The properties are given with proofs. It is not important to know the proofs but to know what the key properties are and have an understanding of why they are important.

Lemma 17.5.1. **Unbiasedness of LSE**
$\hat{}$ is an unbiased estimator of β.

Since $(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T$ is a constant,

$$\begin{aligned} E[\ ] &= E\left[(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{y}\right] \\ &= (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T E[\mathbf{y}]. \end{aligned}$$

Substituting in $\mathbf{Z}\ +\ $ for $\mathbf{y}$

$$\begin{aligned} E[\ ] &= (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T E[\mathbf{Z}\ +\ ] \\ &= (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T(\mathbf{Z}\ + E[\ ]) \\ &= (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T(\mathbf{Z}\ + \mathbf{0}) \\ &= \mathbf{I}_p \\ &= \ . \end{aligned}$$

Lemma 17.5.2. **Variance of LSE**
The variance of$\hat{}$ is given by

$$\mathrm{Var}(\ ) = \sigma^2\left(\mathbf{Z}^T\mathbf{Z}\right)^{-1}.$$

Since for a constant matrix $\mathbf{A}$, we have that $\mathrm{Var}(\mathbf{AY}) = \mathbf{A}\mathrm{Var}(\mathbf{Y})\mathbf{A}^T$, it follows that

$$\begin{aligned} \mathrm{Var}(\ ) &= \mathrm{Var}\left((\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{y}\right) \\ &= (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathrm{Var}(\mathbf{y})\left((\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\right)^T \end{aligned}$$

Substituting in $\mathbf{Z}\ +\ $ for $\mathbf{y}$, and noting that $\mathbf{Z}\ $ is a constant, we have that

$$\begin{aligned} \mathrm{Var}(\ ) &= (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathrm{Var}(\mathbf{Z}\ +\ )\mathbf{Z}(\mathbf{Z}^T\mathbf{Z})^{-1} \\ &= (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathrm{Var}(\ )\mathbf{Z}(\mathbf{Z}^T\mathbf{Z})^{-1} \\ &= (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\sigma^2\mathbf{I}_n\mathbf{Z}(\mathbf{Z}^T\mathbf{Z})^{-1} \\ &= \sigma^2(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{Z}(\mathbf{Z}^T\mathbf{Z})^{-1} \\ &= \sigma^2(\mathbf{Z}^T\mathbf{Z})^{-1}. \end{aligned}$$

Note that Var$\hat{(\ )}$ is the $p \times p$ variance-covariance matrix of the vector$\hat{\ }$. Specifically the i^{th} diagonal entry is $\text{Var}(\hat{\beta}_i)$ and the $(i,j)^{th}$ entry is $\text{Cov}(\hat{\beta}_i, \hat{\beta}_j)$.

Example 17.5.3. **Uncertainty in simple linear regression**
Consider the straight line model:

$$y_i = \alpha + \beta x_i + \epsilon, \qquad i = 1, 2, \ldots, n,$$

where $\epsilon \sim N(0, \sigma^2)$.

Watch Video 25 for a run through uncertainty in the estimates of the parameters of a simple linear regression model. A summary of the results are presented after the video.

Watch Video 25: Uncertainty in simple linear regression

Then

$$\mathbf{Z} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}, \qquad = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}.$$

We have shown in Example 17.4.2 (Simple Linear Regression) that

$$\left(\mathbf{Z}^T\mathbf{Z}\right)^{-1} = \frac{1}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \begin{pmatrix} \frac{1}{n}\sum_{i=1}^{n} x_i^2 & -\bar{x} \\ -\bar{x} & 1 \end{pmatrix}.$$

Therefore,

$$\begin{aligned} \text{Var}\,\hat{(\ )} &= \sigma^2 \left(\mathbf{Z}^T\mathbf{Z}\right)^{-1} \\ &= \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \begin{pmatrix} \frac{1}{n}\sum_{i=1}^{n} x_i^2 & -\bar{x} \\ -\bar{x} & 1 \end{pmatrix}, \end{aligned}$$

and so,

$$\text{Var}(\hat{\alpha}) = \frac{\sigma^2 \sum_{i=1}^{n} x_i^2}{n \sum_{i=1}^{n} (x_i - \bar{x})^2},$$

$$\text{Var}(\hat{\beta}) = \frac{\sigma^2}{\sum_{i=1}^{n} (x_i - \bar{x})^2},$$

$$\text{Cov}(\hat{\alpha}, \hat{\beta}) = \frac{-\sigma^2 \bar{x}}{\sum_{i=1}^{n} (x_i - \bar{x})^2}.$$

The variance of the $\hat{\beta}$ does not depend on the values of α and β but on σ^2 (the variance of ϵ) and the design matrix $\mathbf{Z}$. This tells us that if we have input in choosing x_i (constructing the design matrix) then we can construct the design matrix to reduce the variance of the estimator. In particular, the larger $\sum_{i=1}^{n}(x_i - \bar{x})^2$ (variability in the x_is), the smaller the variance of the estimates. Note that there will often be scientific and practical reasons for choosing x_i within a given range.

Observe that the covariance between $\hat{\alpha}$ and $\hat{\beta}$ has the opposite sign to $\bar{x}$ and becomes larger as $|\bar{x}|$ increases. The correlation between $\hat{\alpha}$ and $\hat{\beta}$ is

$$\text{Cor}(\hat{\alpha}, \hat{\beta}) = \frac{\text{Cov}(\hat{\alpha}, \hat{\beta})}{\sqrt{\text{Var}(\hat{\alpha})\text{Var}(\hat{\beta})}} = \frac{-\sqrt{n}\bar{x}}{\sqrt{\sum_{i=1}^{n} x_i^2}}.$$

The correlation in the estimates is larger, in absolute value, the larger $\bar{x}^2$ is relative to $\sum_{i=1}^{n} x_i^2$.

To illustrate the variability in $\hat{\beta}$ we use an example. Suppose that we have ten observations from the model:

$$y = 2 + 0.6x + \epsilon$$

where $\epsilon \sim N(0, 1)$ and for $i = 1, 2, \ldots, 10$, $x_i = i$.

Then

$$\begin{aligned}\text{Var}(\hat{\beta}) &= \frac{1}{\sum_{i=1}^{n}(x_i-\bar{x})^2}\begin{pmatrix}\frac{1}{n}\sum_{i=1}^{n}x_i^2 & -\bar{x}\\ -\bar{x} & 1\end{pmatrix}\\ &= \frac{1}{82.5}\begin{pmatrix}38.5 & -5.5\\ -5.5 & 1\end{pmatrix}\\ &= \begin{pmatrix}0.46667 & -0.06667\\ -0.06667 & 0.01212\end{pmatrix}\end{aligned}$$

We simulated 100 sets of data from the model and for each set of data calculate $\hat{\alpha}$ and $\hat{\beta}$. In Figure 17.1, the estimates of $\hat{\beta}$ against $\hat{\alpha}$ are plotted along with the true parameter values $\beta = 0.6$ and $\alpha = 2$. The estimates show negative correlation.

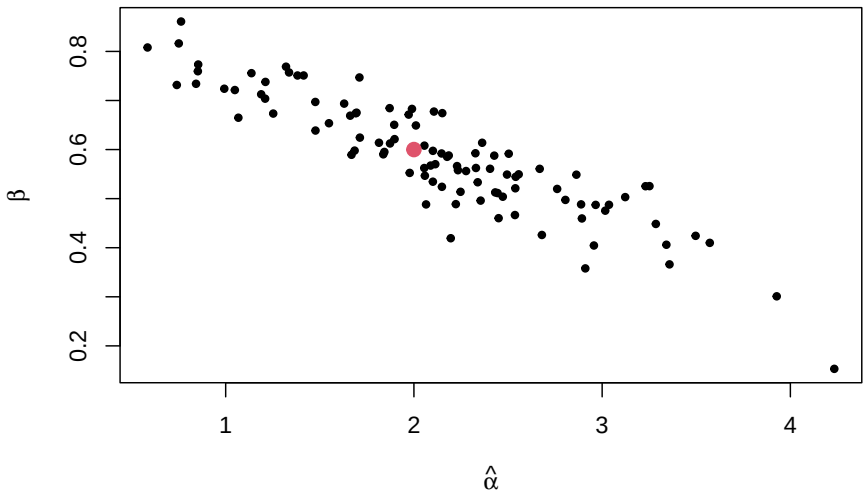


Figure 17.1: Plot of estimates of straight line model parameters with true parameter values denoted by a red dot

In Figure 17.2, the fitted line $\hat{\alpha}+\hat{\beta}x$ is plotted for each simulated data set along with the true line $2 + 0.6x$. Observe that the lines with the highest intercepts tend to have the smallest slope and visa-versa. Also note that there is more variability in the estimated lines at the end points ($x = 1$ and $x = 10$) rather than in the middle of the range (close to $x = 5.5$).

Lemma 17.5.4. **Distribution of LSE**

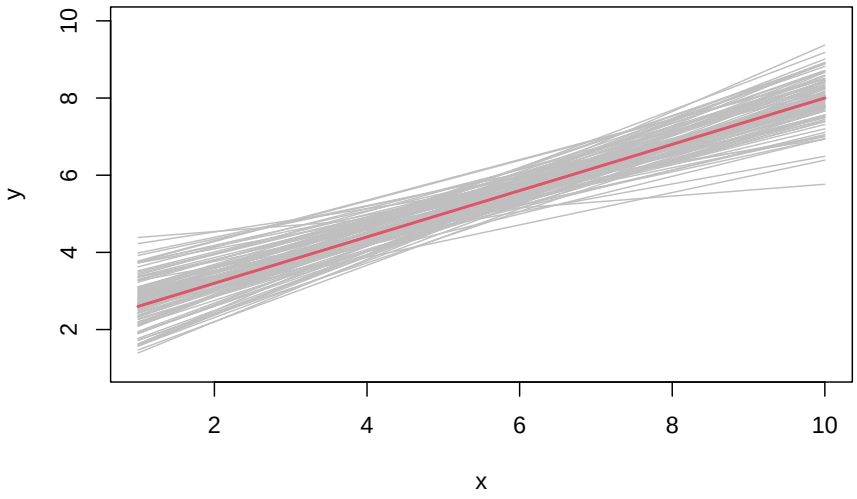


Figure 17.2: Estimated lines from 100 simulations with true line in red

If additionally $\sim N_n(\mathbf{0}, \sigma^2\mathbf{I}_n)$, then

$$\hat{} \sim N_p\left(, \sigma^2(\mathbf{Z}^T\mathbf{Z})^{-1}\right).$$

Note,

$$\begin{aligned}
\hat{} &= (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{y} \\
&= (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T(\mathbf{Z} \ + \ ) \\
&= (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{Z} \ + (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T \\
&= \ + (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T \ .
\end{aligned}$$

Hence$\hat{}$ is a linear function of a normally distributed random variable. Using the identities $E[A\mathbf{x} + b] = AE[\mathbf{x}] + b$ and $\text{Var}(A\mathbf{x} + b) = A\text{Var}(\mathbf{x})A^T$, consequently $\hat{}$ has a normal distribution with mean and variance as required.

Note that since$\hat{} \sim N_p(\ , \sigma^2(\mathbf{Z}^T\mathbf{Z})^{-1})$, then each of the individual parameters has a distribution

$$\hat{\beta}_i \sim N\left(\beta_i, \sigma^2((\mathbf{Z}^T\mathbf{Z})^{-1})_{ii}\right),$$

However the individual $\hat{\beta}_i$ are not independent as we saw in Example 17.5.3 (Uncertainty in simple linear regression).

17.6 Gauss-Markov Theorem

The Gauss-Markov Theorem shows that a good choice of estimator for $\mathbf{a}^T\beta$, a linear combination of the parameters, is $\mathbf{a}^{\mathcal{T}\hat{}}$.

Theorem 17.6.1. **Gauss-Markov Theorem**
If$\hat{}$ is the least squares estimator of , then $\mathbf{a}^{\mathcal{T}\hat{}}$ is the *unique linear unbiased estimator* of $\mathbf{a}^T$ with minimum variance.

The details of the proof of Theorem 17.6.1 (Gauss-Markov Theorem) are provided but can be omitted.

Proof of Gauss-Markov Theorem.

Consider$\hat{}$ $= (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{y}$, the LSE of . Hence,

$$\mathbf{a}^{\mathcal{T}\hat{}} = \mathbf{a}^T(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{y} = \mathbf{C}\mathbf{y},$$

where $\mathbf{C} = \mathbf{a}^T(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T$. It follows that $\mathbf{a}^{\mathcal{T}\hat{}}$ is a linear function of $\mathbf{y}$.

Note that $\mathbf{a}^{\mathcal{T}\hat{}}$ is an unbiased estimator of $\mathbf{a}^T$ because,

$$\begin{aligned} E[\mathbf{a}^{\mathcal{T}\hat{}}] &= E[\mathbf{C}\mathbf{y}] \\ &= \mathbf{C}E[\mathbf{Z} +] \\ &= \mathbf{C}\mathbf{Z} + \mathbf{C}E[ ] \\ &= \mathbf{a}^T(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{Z} + \mathbf{0} \\ &= \mathbf{a}^T . \end{aligned}$$

Suppose there exists another linear unbiased estimator of $\mathbf{a}^T$, denoted $\mathbf{b}^T\mathbf{y}$. By definition

$$E[\mathbf{b}^T\mathbf{y}] = \mathbf{a}^T .$$

However we can also calculate

$$\begin{aligned} E[\mathbf{b}^T\mathbf{y}] &= \mathbf{b}^T E[\mathbf{Z}\ +\ ] \\ &= \mathbf{b}^T\mathbf{Z}\ . \end{aligned}$$

It follows that

$$\mathbf{b}^T\mathbf{Z}\ = \mathbf{a}^T\ , \qquad \text{for all}\ \ ,$$

so

$$\mathbf{a}^T = \mathbf{b}^T\mathbf{Z}.$$

Now

$$\begin{aligned} \mathrm{Var}(\mathbf{b}^T\mathbf{y}) &= \mathbf{b}^T\mathrm{Var}(\mathbf{Z}\ +\ )\mathbf{b} \\ &= \mathbf{b}^T\mathrm{Var}(\ )\mathbf{b} \\ &= \mathbf{b}^T\sigma^2\mathbf{I}_n\mathbf{b} = \sigma^2\mathbf{b}^T\mathbf{b}, \end{aligned}$$

and

$$\begin{aligned} \mathrm{Var}(\mathbf{a}^{\mathcal{P}}) &= \mathrm{Var}(\mathbf{C}\mathbf{y}) \\ &= \mathbf{C}\mathrm{Var}(\mathbf{Z}\ +\ )\mathbf{C}^T \\ &= \mathbf{C}\mathrm{Var}(\ )\mathbf{C}^T \\ &= \mathbf{C}\sigma^2\mathbf{I}_n\mathbf{C}^T \\ &= \sigma^2\mathbf{C}\mathbf{C}^T \\ &= \sigma^2(\mathbf{a}^T(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T)(\mathbf{a}^T(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T)^T \\ &= \sigma^2\mathbf{a}^T(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{Z}(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{a} \\ &= \sigma^2\mathbf{a}^T(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{a}. \end{aligned}$$

Substituting $\mathbf{a}^T = \mathbf{b}^T\mathbf{Z}$, we can rewrite

$$\begin{aligned} \mathrm{Var}(\mathbf{a}^{\mathcal{P}}) &= \sigma^2\mathbf{b}^T\mathbf{Z}(\mathbf{Z}^T\mathbf{Z})^{-1}(\mathbf{b}^T\mathbf{Z})^T \\ &= \sigma^2\mathbf{b}^T\mathbf{Z}(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{b} \\ &= \sigma^2\mathbf{b}^T\mathbf{P}\mathbf{b}. \end{aligned}$$

Comparing $\text{Var}(\mathbf{b}^T\mathbf{y})$ and $\text{Var}(\mathbf{a}^{\mathcal{P}_{\mathcal{K}}})$, we get

$$\begin{aligned}
\text{Var}(\mathbf{b}^T\mathbf{y}) - \text{Var}(\mathbf{a}^{\mathcal{P}_{\mathcal{K}}}) &= \sigma^2\mathbf{b}^T\mathbf{b} - \sigma^2\mathbf{b}^T\mathbf{P}\mathbf{b} \\
&= \sigma^2\mathbf{b}^T(\mathbf{I}_n - \mathbf{P})\mathbf{b} \\
&= \sigma^2\mathbf{b}^T(\mathbf{I}_n - \mathbf{P})^2\mathbf{b} \\
&= \sigma^2\mathbf{b}^T(\mathbf{I}_n - \mathbf{P})^T(\mathbf{I}_n - \mathbf{P})\mathbf{b} \\
&= \sigma^2\mathbf{D}^T\mathbf{D},
\end{aligned}$$

where $\mathbf{D} = (\mathbf{I}_n - \mathbf{P})\mathbf{b}$. Therefore,

$$\text{Var}(\mathbf{b}^T\mathbf{y}) - \text{Var}(\mathbf{a}^{\mathcal{P}_{\mathcal{K}}}) = \sigma^2\mathbf{D}^T\mathbf{D} \geq 0,$$

so $\mathbf{a}^{\mathcal{P}_{\mathcal{K}}}$ has the smallest variance of any other linear unbiased estimator.

Finally suppose that $\mathbf{b}^T\mathbf{y}$ is another linear unbiased estimator such that $\text{Var}(\mathbf{b}^T\mathbf{y}) = \text{Var}(\mathbf{a}^{\mathcal{P}_{\mathcal{K}}})$, then

$$\begin{aligned}
&\text{Var}(\mathbf{b}^T\mathbf{y}) - \text{Var}(\mathbf{a}^{\mathcal{P}_{\mathcal{K}}}) = \sigma^2\mathbf{D}^T\mathbf{D} = 0 \\
&\qquad\Longrightarrow \qquad \mathbf{D} = \mathbf{0}
\end{aligned}$$

Since $\mathbf{D} = (\mathbf{I}_n - \mathbf{P})\mathbf{b} = \mathbf{0}$, it follows that

$$\begin{aligned}
\mathbf{b} &= \mathbf{P}\mathbf{b} \\
&= \mathbf{Z}(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{b} \\
&= \mathbf{Z}(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{a} \\
\Longrightarrow \qquad \mathbf{b}^T &= \mathbf{a}^T(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T,
\end{aligned}$$

So

$$\begin{aligned}
\mathbf{b}^T\mathbf{y} &= \mathbf{a}^T(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{y} \\
&= \mathbf{a}^{\mathcal{P}_{\mathcal{K}}}.
\end{aligned}$$

Therefore $\mathbf{a}^{\mathcal{P}_{\mathcal{K}}}$ is the *unique linear unbiased estimator* of $\mathbf{a}^T$.

Theorem 17.6.2. **Best linear unbiased estimator (BLUE)**
If $\mathbf{a}^T = (0, 0, \dots, 1, 0, \dots, 0)$ where the 1 is in the ith position, then $\hat{\beta}_i$ is the *best linear unbiased estimator*, shorthand BLUE, of β_i.

The following **R shiny** app generates data and fits a regression line, $y = \alpha + \beta x$. It allows for variability in the coefficients and how the covariates x are generated. Predicted values can also be plotted with confidence intervals, see Section 18, Interval Estimation for an introduction to confidence intervals and Lab 12: Linear Models II for a discussion of confidence intervals for predicted values.

R Shiny app: Linear Model

Task: Session 9

Attempt the **R Markdown** file for Session 9:
Session 9: Linear Models I

Student Exercises

Attempt the exercises below.

Exercise 17.1.
Suppose that a model states that

$$E[Y_1] = \theta, \qquad E[Y_2] = 2\theta - \phi, \qquad E[Y_3] = \theta + 2\phi.$$

Find the least squares estimates of θ and ϕ.

Exercise 17.2.

The marks of 8 students are presented below. For student i, x_i denotes their mark in a mid-term test and y_i denotes their mark in the final exam.

Mid-term test marks:

$$\mathbf{x} = (x_1, x_2, \dots, x_8) = (75, 68, 60, 58, 70, 67, 64, 65)$$

Final exam marks:

$$\mathbf{y} = (y_1, y_2, \dots, y_8) = (62, 54, 55, 43, 59, 59, 56, 50).$$

Note that:

$$
\begin{aligned}
\bar{x} &= \frac{1}{8}\sum_{i=1}^{8} x_i = 65.875 \\
\bar{y} &= \frac{1}{8}\sum_{i=1}^{8} y_i = 54.75 \\
s_{xy} &= \frac{1}{8-1}\left\{\sum_{i=1}^{8} x_i y_i - n\bar{x}\bar{y}\right\} = 25.679 \\
s_x^2 &= \frac{1}{8-1}\left\{\sum_{i=1}^{8} x_i^2 - n\bar{x}^2\right\} = 29.554 \\
s_y^2 &= \frac{1}{8-1}\left\{\sum_{i=1}^{8} y_i^2 - n\bar{y}^2\right\} = 35.929
\end{aligned}
$$

(a) Calculate the correlation between the mid-term test marks and the final exam marks.

(b) Fit a straight line linear model $y = \alpha + \beta x + \epsilon$, where $\epsilon \sim N(0, \sigma^2)$ with the final exam mark, y, as the response and the mid-term test mark, x, as the predictor variable. Include estimation of σ^2 in the model fit.

(c) Find the expected final exam mark of a student who scores 79 in the mid-term test.

Chapter 18

Interval Estimation

18.1 Introduction

In this section, we will explore the concept of an interval estimate. We have seen how the Method of Moments, Maximum Likelihood Estimation and Least Squares can be used to find *point* estimates of parameters. These estimates often have desirable properties such as unbiasedness (the average value of the sample estimate of the parameter is the true population parameter) and consistency (the sample estimate of the parameter converges to the true population parameter as the sample size tends to infinity). However, for finite samples our sample estimate of the parameter will rarely be equal to the true population parameter. Therefore we construct interval estimates, which allow us to quantify our (un)certainty about parameters.

We start with an exercise for you to attempt to construct intervals which you believe contain the true answer. This will provide motivation for the construction of **confidence intervals**.

18.2 Confident?

The board game **Confident?** gets players to give an interval for a numerical answer.

The player with the **shortest** interval containing the **correct** answer wins a point.

Do you think you would be good at this?

Attempt the following four questions: Confident? Questions

After you have attempted the questions, watch Video 26 for the answers. The video includes discussion of steps for constructing intervals and how we begin

to construct confidence intervals.

Watch Video 26: Confident?

18.3 Confidence intervals

If we are interested in estimating a given parameter θ we can find some estimator $T(\mathbf{X})$ using some appropriate method, for example Method of Moments, Maximum Likelihood Estimation or Least Squares Estimation. $T(\mathbf{X})$ is called a point estimator since the estimate of θ that we report is one particular point in the parameter space.

For example, when we are interested in estimating the percentage of UK residents who are in favour of the Government's policies, we can collect a random sample of UK residents and compute the sample proportion of the people in favour of the policies. We then report that the Government has, say, a 54% approval rating.

The difficulty that arises, though, is what does 54% mean? How exact is our estimate? The point estimator does not give us that information. Instead it is helpful to also include information about the variability of the estimate given, and that will depend both upon the true underlying variance of the population and the sampling distribution of the estimator that we use.

We have 2 options:

1. Report the value of the estimate and the standard deviation of the estimate, which is often called the **standard error** of the estimate. For example, the Government has a 54% approval rating with a 2% standard error.

2. Construct an interval estimate for the parameter which incorporates both information about the point estimate, its standard error, and the sampling distribution of the estimator. For example, a 95% confidence interval for the Government's approval rating is 52.4% to 55.6%.

Definition 18.3.1. **Confidence Interval**

Let $\alpha \in [0, 1]$ be a fixed value. A $100(1-\alpha)\%$ *confidence interval* for the parameter θ is an interval constructed from a random sample such that if we were to repeat the experiment a large number of times the interval would contain the true value of θ in $100(1-\alpha)\%$ of the cases.

Note that the interval will depend on the value of the estimate and the sampling distribution of the estimator.

Example 18.3.2.
Suppose that $x_1, x_2, \ldots, x_n$ is a random sample from a normal distribution with

mean θ and known variance σ_0^2. Construct a $100(1-\alpha)\%$ confidence interval for θ.

Watch Video 27 for the construction of the confidence interval for θ.

Watch Video 27: Confidence interval for θ

Construction of confidence interval for θ.

First, we need a point estimator for θ, the mean of the normal distribution. The Method of Moments estimator and MLE for θ are both $\hat{\theta} = \bar{x}$, the sample mean.

Next we determine the sampling distribution of the estimator $\hat{\theta}$. Since $X_1, X_2, \ldots, X_n$ is a random sample from a normal distribution, it follows that

$$\hat{\theta} = \frac{1}{n}\sum_{i=1}^{n} X_i = \bar{X} \sim N\left(\theta, \frac{\sigma_0^2}{n}\right).$$

We want to find endpoints $\hat{\theta}_1$ and $\hat{\theta}_2$ such that

$$P\left(\hat{\theta}_1 \leq \theta \leq \hat{\theta}_2\right) = 1 - \alpha.$$

Note that $\hat{\theta}_1$ and $\hat{\theta}_2$ are random values which are determined by the random sample.

Note that there exist an infinite number of $100(1-\alpha)\%$ confidence intervals for θ. We would like to chose the one that is *best*, that is, the one for which the length of the interval $\hat{\theta}_2 - \hat{\theta}_1$ is the shortest. This will be the interval which is symmetric around θ if the distribution of $\hat{\theta}$ is symmetric.

Since $\hat{\theta} = \bar{X} \sim N\left(\theta, \frac{\sigma_0^2}{n}\right)$, if we standardise, then we can obtain the normal distribution

$$\frac{\bar{X} - \theta}{\sigma_0/\sqrt{n}} \sim N(0,1)$$

and so

$$P\left(-z_{\alpha/2} \leq \frac{\bar{X} - \theta}{\sigma_0/\sqrt{n}} \leq z_{\alpha/2}\right) = 1 - \alpha,$$

where z_β satisfies $P(Z > z_\beta) = \beta$. The symmetry of the normal distribution means that also $P(Z < -z_\beta) = \beta$.

Solving for θ we get,

$$P\left(-z_{\alpha/2}\cdot\frac{\sigma_0}{\sqrt{n}}\leq\bar{X}-\theta\leq z_{\alpha/2}\cdot\frac{\sigma_0}{\sqrt{n}}\right)=1-\alpha$$
$$P\left(-\bar{X}-z_{\alpha/2}\cdot\frac{\sigma_0}{\sqrt{n}}\leq-\theta\leq-\bar{X}+z_{\alpha/2}\cdot\frac{\sigma_0}{\sqrt{n}}\right)=1-\alpha$$
$$P\left(\bar{X}-z_{\alpha/2}\cdot\frac{\sigma_0}{\sqrt{n}}\leq\theta\leq\bar{X}+z_{\alpha/2}\cdot\frac{\sigma_0}{\sqrt{n}}\right)=1-\alpha$$

Therefore, a $100(1-\alpha)\%$ confidence interval for θ, where θ is the mean of a normal distribution with known variance σ_0^2 is

$$\left(\bar{x}-z_{\alpha/2}\cdot\frac{\sigma_0}{\sqrt{n}},\bar{x}+z_{\alpha/2}\cdot\frac{\sigma_0}{\sqrt{n}}\right).$$

Example 18.3.3.
Suppose that $x_1, x_2, \ldots, x_n$ is a random sample from a normal distribution with mean θ and unknown variance σ^2. Construct a $100(1-\alpha)\%$ confidence interval for θ.

Again we use $\hat{\theta}=\bar{x}$, since $\bar{x}$ is the minimum variance unbiased estimator of θ.

We know that $\bar{X}\sim N\left(\theta,\frac{\sigma^2}{n}\right)$, so

$$\frac{\bar{X}-\theta}{\sigma/\sqrt{n}}\sim N(0,1),$$

but now the variance σ^2 is unknown. Hence if we want to find the confidence interval for θ, we need to estimate σ. It is known that $\frac{\bar{X}-\theta}{s/\sqrt{n}}\sim t_{n-1}$ where s^2 is the sample variance. Therefore

$$P\left(-t_{n-1,\alpha/2}\leq\frac{\bar{X}-\theta}{s/\sqrt{n}}\leq t_{n-1,\alpha/2}\right)=1-\alpha.$$

Isolating θ we get,

$$P\left(\bar{X}-t_{n-1,\alpha/2}\cdot\frac{s}{\sqrt{n}}\leq\theta\leq\bar{X}+t_{n-1,\alpha/2}\cdot\frac{s}{\sqrt{n}}\right)=1-\alpha.$$

Therefore a $100(1-\alpha)\%$ confidence interval for θ, where θ is the mean of the normal distribution with unknown variance σ^2, is given by

$$\left(\bar{x} - t_{n-1,\alpha/2}\frac{s}{\sqrt{n}}, \bar{x} + t_{n-1,\alpha/2} \cdot \frac{s}{\sqrt{n}}\right).$$

We make a few observations about the confidence intervals constructed in Example 18.3.2 and Example 18.3.3

- The sample mean $\bar{x}$ (maximum likelihood estimator/method of moments estimator) is contained in our confidence intervals and in these cases the confidence interval is symmetric about $\bar{x}$.

- The confidence intervals become smaller with n. That is, the more data (information) we have, the smaller the confidence interval becomes. Specifically, the confidence intervals decrease at rate $1/\sqrt{n}$. Therefore if we increase the sample size to $4n$ we will (approximately) half the length of the confidence interval. The exact impact on the confidence interval will depend on the sample mean, and if the variance is unknown, sample variance.

- As α becomes smaller, $z_{\alpha/2}$ ($t_{n-1,\alpha/2}$) and $1-\alpha$ become larger. That is, the width of the confidence interval increases as we increase the level of confidence. We will explore in Session 10: Confidence intervals and hypothesis testing the effect of α on the confidence interval.

- The t-distribution has *fatter* tails than the normal distribution and has *fatter* tails for smaller values of n. Mathematically, for any $0 < \alpha < 1$ and for any $n < m$, we have that

  $$z_{\alpha/2} < t_{m-1,\alpha/2} < t_{n-1,\alpha/2}.$$

  That is, the confidence intervals are wider the smaller n is in the case of an unknown variance. This is a consequence of us being less certain about the population variance for smaller values of n. Note that as $n \to \infty$, $t_{n-1,\alpha/2} \to z_{\alpha/2}$ as the uncertainty in the variance decreases.

18.4 Asymptotic distribution of the MLE

Let $\hat{\theta}$ be the MLE of θ. Recall that $\hat{\theta} \to N\left(\theta, \frac{1}{I(\theta)}\right)$ as $n \to \infty$. Consequently we can construct an approximate $100(1-\alpha)\%$ confidence interval for θ, however since θ is unknown we will also need to approximate $\frac{1}{I(\theta)}$ with the observed information

$$I_0(\hat{\theta}) = E\left[-\frac{d^2 l(\theta)}{d\theta^2}\right]\Bigg|_{\theta=\hat{\theta}}.$$

Consequently,

$$P\left(-z_{\alpha/2} \leq \frac{\hat{\theta}-\theta}{\sqrt{\frac{1}{I_0(\hat{\theta})}}} \leq z_{\alpha/2}\right) = 1-\alpha,$$

and an approximate $100(1-\alpha)\%$ confidence interval for θ is given by

$$\left(\hat{\theta} - z_{\alpha/2}\sqrt{\frac{1}{I_0(\hat{\theta})}}, \hat{\theta} + z_{\alpha/2}\sqrt{\frac{1}{I_0(\hat{\theta})}}\right).$$

This method is extremely useful since it is often quite straightforward to evaluate the MLE and the observed information. Nonetheless it is an approximation, and should only be trusted for large values of n, though the quality of the approximation will vary from model to model.

Example 18.4.1.
Consider $Y_1, Y_2, \ldots, Y_n \sim \text{Exp}(\theta^{-1})$ independently. Construct an approximate 95% confidence interval for θ.

For each of the Y_i, some $y_i > 0$ is observed and we have

$$f(y_i|\theta) = \theta^{-1}e^{-y_i/\theta}.$$

Thus calculating the likelihood and log-likelihood functions:

$$\begin{aligned} L(\theta) &= \prod_{i=1}^{n} f(y_i|\theta) \\ &= \theta^{-n} e^{-\sum_{i=1}^{n} y_i/\theta} \\ l(\theta) &= -n\log\theta - \sum_{i=1}^{n}\frac{y_i}{\theta} \end{aligned}$$

which is maximised by

$$\hat{\theta} = \sum_{i=1}^{n}\frac{y_i}{n} = \bar{y}.$$

Now,

$$\frac{d^2 l(\theta)}{d\theta^2} = \frac{n}{\theta^2} - \frac{2\sum_{i=1}^{n} y_i}{\theta^3}$$

so that

$$I_0(\hat{\theta}) = -\left(\frac{n}{\bar{y}^2} - \frac{2n\bar{y}}{\bar{y}^3}\right) = \frac{n}{\bar{y}^2}.$$

Hence, an approximate 95% confidence interval for θ is

$$\left(\bar{y} - 1.96 \times \sqrt{\frac{\bar{y}^2}{n}}, \bar{y} + 1.96 \times \sqrt{\frac{\bar{y}^2}{n}}\right) = \bar{y}\left(1 - \frac{1.96}{\sqrt{n}}, 1 + \frac{1.96}{\sqrt{n}}\right).$$

Example 18.4.2.
Consider $Y_1, Y_2, \ldots, Y_n \sim N(\theta, 1)$ independently. Construct an approximate 95% confidence interval for θ.

As noted in Section 10.3, Example 10.3.7, we showed that $\hat{\theta} = \bar{y}$ and

$$\frac{d^2 l(\theta)}{d\theta^2} = -n.$$

Hence, $I_0(\hat{\theta}) = n$, and a 95% confidence interval for θ is

$$\left(\bar{y} - 1.96 \times \sqrt{\frac{1}{n}}, \bar{y} + 1.96 \times \sqrt{\frac{1}{n}}\right).$$

Note that the confidence interval constructed in Example 18.4.2 coincides with the confidence interval constructed in Example 18.3.2 with $\sigma_0^2 = 1$. This is because the MLE, $\hat{\theta}$, satisfies $\hat{\theta} = \bar{Y} \sim N(\theta, 1/n)$.

Chapter 19

Hypothesis Testing

19.1 Introduction to hypothesis testing

In estimation, we are interested in asking ourselves the question what is the value of some particular parameter of interest in the population. For example, what is the average annual income of residents in the UK?

Often there are times in statistics when we are not interested in the specific value of the parameter, but rather are interested in asserting some statement regarding the parameter of interest. Some examples:

- We want to claim that the average annual income of UK residents is more than or equal to £35,000.
- We want to assess whether the average annual income of men in academia in the UK is the same as that of women in similar ranks.
- We want to determine whether the number of cars crossing a certain intersection follows a Poisson distribution or whether it is more likely to come from a geometric distribution.

To perform a statistical hypothesis test, one needs to specify two disjoint hypotheses in terms of the parameters of the distribution that are of interest. They are

- H_0 : Null Hypothesis,
- H_1 : Alternative Hypothesis.

Traditionally, we choose H_0 to be the claim that we would like to assert.

Returning to our examples:

- We want to claim that the average annual income of UK residents is more than or equal to £35,000. We test

$$H_0 : \mu \geq 35,000 \quad \text{vs.} \quad H_1 : \mu < 35,000.$$

- We want to assess whether the average annual income of men in academia in the UK is the same as that of women at similar ranks. We test

$$H_0 : \mu_{\text{men}} = \mu_{\text{women}} \quad \text{vs.} \quad H_1 : \mu_{\text{men}} \neq \mu_{\text{women}}.$$

- We want to determine whether the number of cars crossing a certain intersection follows a Poisson distribution or whether it is more likely to come from a geometric distribution. We test

$$H_0 : X \sim \text{Po}(2) \quad \text{vs.} \quad H_1 : X \sim \text{Geom}(0.5).$$

Hypotheses where the distribution is completely specified are called simple hypotheses. For example, H_0 and H_1 in the car example and H_0 in the gender wage example are all simple hypotheses.

Hypotheses where the distribution is not completely specified are called composite hypotheses. For example, H_0 and H_1 in the average annual income example and H_1 in the gender wage example are all composite hypotheses.

Note that in the average annual income and gender wage examples, the null and alternative hypotheses cover all possibilities, whereas for the car example there are many other choices of distributions which could be hypothesized.

Definition 19.1.1. **The conclusion of a hypothesis test**
We will **reject** H_0 if there is sufficient information from our sample that indicates that the null hypothesis cannot be true thereby concluding the alternative hypothesis is true.

We will **not reject** H_0 if there is not sufficient information in the sample to refute our claim.

The remainder of this section is structured as follows. We define Type I and Type II errors, which are the probability of making the wrong decision in a hypothesis test. In Section 19.3 we show how to construct hypothesis tests starting with hypothesis tests for the mean of a normal distribution with known variance. This is extended to the case where the variance is unknown and where we have two samples we want to compare. We introduce p-values which give a measure of how likely (unlikely) the observed data are if the null hypothesis is true.We then consider hypothesis testing in a wide range of scenarios:-

- Normal means with unknown variance
- Confidence intervals and two-sided tests

- Distribution of Variance
- Other types of hypothesis tests
- Sample size calculations

19.2 Type I and Type II errors

Definition 19.2.1. **Type I error**
A *Type I error* occurs when one chooses to incorrectly reject a true null hypothesis.

A Type I error is also commonly referred to as a *false positive*.

Definition 19.2.2. **Type II error**
A *Type II error* occurs when one fails to reject a false null hypothesis.

A Type II error is also commonly referred to as a *false negative*.

Type I error and Type II error are summarised in the following decision table.

	One accepts the Null	One rejects the Null
Null hypothesis is true	Correct Conclusion	Type I Error
Null hypothesis is false	Type II Error	Correct Conclusion

Definition 19.2.3. **Significance level**
The *significance level* or *size* of the test is

$$\begin{aligned}\alpha &= P(\text{Type I error}) \\ &= P(\text{Reject } H_0 | H_0 \text{ true}).\end{aligned}$$

Typical choices for α are 0.01, 0.05 and 0.10.

Definition 19.2.4. **Probability of Type II error**
The probability of a Type II error is

$$\begin{aligned}\beta &= P(\text{Type II error}) \\ &= P(\text{Do Not Reject } H_0 | H_1 \text{ true}).\end{aligned}$$

Consider the following properties of α and β:

- It can be shown that there is an inverse relationship between α and β, that is as α increases, β decreases and vice versa. Therefore for a fixed sample size one can only choose to control one of the types of error. In hypothesis testing we choose to control Type I error and select our hypotheses initially so the "worse" error is the Type II error.

- The value of both α and β depend on the value of the underlying parameters. Consequently, we can control α by first choosing H_0 to include an equality of the parameter, and then showing that the largest the Type I error can be is at this point of equality. Therefore we may as well choose the parameter to be the size. To illustrate in the average annual income example above

$$\begin{aligned}\alpha &= P(\text{rejecting } H_0 | \mu = 35,000) \\ &\geq P(\text{rejecting } H_0 | \mu \geq 35,000).\end{aligned}$$

  Therefore $H_0 : \mu \geq 35,000$ is often just written as $H_0 : \mu = 35,000$.

- Because H_0 describes an equality, H_1 is therefore a composite hypothesis. Therefore $\beta = P(\text{Type II error})$ is a function of the parameter within the alternative parameter space.

Definition 19.2.5. **Power of a Test**
The *power* of the test is

$$\begin{aligned}1 - \beta &= 1 - P(\text{Type II error}) \\ &= P(\text{Reject } H_0 | H_1 \text{ true}).\end{aligned}$$

The power of a test can be thought of as the probability of making a correct decision.

19.3 Tests for normal means, σ known

In this section we study a number of standard hypothesis tests that one might perform on a random sample.

We assume throughout this section that $x_1, x_2, \ldots, x_n$ are i.i.d. samples from X with $E[X] = \mu$, where μ is unknown and $var(X) = \sigma^2$ is known.

Test 1: $H_0 : \mu = \mu_0$ vs. $H_1 : \mu < \mu_0$; σ^2 known.

Watch Video 28 for the construction Hypothesis Test 1.

Watch Video 28: Hypothesis Test 1

A summary of the construction of Hypothesis Test 1 is given below.

Data assumptions. We assume either

- $X_1, X_2, \ldots, X_n$ are a random sample from a normal distribution with known variance σ^2;
- The sample size n is sufficiently large so that we can assume $\bar{X}$ is approximately normally distributed by the Central Limit Theorem, and that either the variance is known or that the sample variance $s^2 \approx \sigma^2$.

Step 1: Choose a **test statistic** based upon the random sample for the parameter we want to base our claim on. For example, we are interested in μ so we want to choose a good estimator of μ as our test statistic. That is, $\hat{\mu} = \bar{X}$.

Step 2: Specify a **decision rule**. The smaller $\bar{X}$ is, the more the evidence points towards the alternative hypothesis $\mu < \mu_0$. Therefore our decision rule is to reject H_0 if $\bar{X} < c$, where c is called the **cut-off** value for the test.

Step 3: Based upon the sampling distribution of the test statistic and the specified significance level of the test, solve for the specific value of the **cut-off** value c. To find c,

$$\begin{aligned}
\alpha &= P(\text{Type I error}) \\
&= P(\text{Reject } H_0 | H_0 \text{ true}) \\
&= P(\bar{X} < c | \mu = \mu_0) \\
&= P\left(\bar{X} < c | \bar{X} \sim N\left(\mu_0, \frac{\sigma^2}{n}\right)\right) \\
&= P\left(\frac{\bar{X} - \mu_0}{\sigma/\sqrt{n}} < \frac{c - \mu_0}{\sigma/\sqrt{n}}\right) \\
&= P\left(Z < \frac{c - \mu_0}{\sigma/\sqrt{n}}\right).
\end{aligned}$$

Since $P(Z < -z_\alpha) = \alpha$, where z_α can be found using `qnorm(1-alpha)` ($P(Z < z_\alpha) = 1 - \alpha$) or statistical tables, then

$$-z_\alpha = \frac{c - \mu_0}{\sigma/\sqrt{n}}$$

and $c = \mu_0 - z_\alpha \cdot \frac{\sigma}{\sqrt{n}}$.

So, the **decision rule** is to reject H_0 if $\bar{X} < \mu_0 - z_\alpha \cdot \frac{\sigma}{\sqrt{n}}$ or, equivalently,

$$Z = \frac{\bar{X} - \mu_0}{\sigma\sqrt{n}} < -z_\alpha.$$

Test 2: $H_0 : \mu = \mu_0$ vs. $H_1 : \mu < \mu_0$; σ^2 known.

This is similar to the previous test, except the **decision rule** is to reject H_0 if $\bar{X} > \mu_0 + z_\alpha \frac{\sigma}{\sqrt{n}}$ or, equivalently,

$$Z = \frac{\bar{X} - \mu_0}{\sigma/\sqrt{n}} > z_\alpha.$$

Note that both these tests are called **one-sided tests**, since the rejection region falls on only one side of the outcome space.

Test 3: $H_0 : \mu = \mu_0$ vs. $H_1 : \mu \neq \mu_0$; σ^2 known.

The test statistic $\bar{X}$ does not change but the decision rule will. The **decision rule** is to reject H_0 if $\bar{X}$ is sufficiently far (above or below) from μ_0. Specifically, reject H_0 if $\bar{X} < \mu_0 - z_{\alpha/2} \cdot \frac{\sigma}{\sqrt{n}}$ or $\bar{X} > \mu_0 + z_{\alpha/2} \cdot \frac{\sigma}{\sqrt{n}}$. Equivalent to both of these is

$$|Z| = \left| \frac{\bar{X} - \mu_0}{\sigma/\sqrt{n}} \right| > z_{\alpha/2}.$$

This is called a **two-sided test** because the decision rule partitions the outcome space into two disjoint intervals.

Example 19.3.1. **Coffee machine.**
Suppose that a coffee machine is designed to dispense 6 ounces of coffee per cup with a standard deviation $\sigma = 0.2$, where we assume the amount of coffee dispensed is normally distributed. A random sample of $n = 20$ cups gives $\bar{x} = 5.94$.Test whether the machine is correctly filling the cups.

We test $H_0 : \mu = 6.0$ vs. $H_1 : \mu \neq 6.0$ at significance level $\alpha = 0.05$.

Using a two-sided test with known variance, the decision rule is to reject H_0 if $|Z| = \left| \frac{\bar{x} - 6.0}{0.2/\sqrt{20}} \right| > z_{0.05/2} = z_{0.025} = 1.96$. Now

$$|Z| = \left| \frac{5.94 - 6.0}{0.2/\sqrt{20}} \right| = |-1.34| < 1.96.$$

Therefore, we conclude that there is not enough statistical evidence to reject H_0 at $\alpha = 0.05$.

19.4 p values

When our sample information determines a particular conclusion to our hypothesis test, we only report that we either reject or do not reject H_0 at a particular

significance level α. Hence when we report our conclusion the reader doesn't know how sensitive our decision is to the choice of α.

To illustrate, in Example 19.3.1 (Coffee Machine) we would have reached the same conclusion that there is not enough statistical evidence to reject H_0 at $\alpha = 0.05$ if $|Z| = 1.95$ rather than $|Z| = 1.34$. Whereas, if the significance level was $\alpha = 0.10$, we would have rejected H_0 if $|Z| = 1.95 > z_{0.10/2} = 1.6449$, but we would not reject H_0 if $|Z| = 1.34 < z_{0.10/2} = 1.6449$.

Note that the choice of α should be made before the test is performed; otherwise, we run the risk of inducing experimenter bias!

Definition 19.4.1. ***p*-value**
The *p-value* of a test is the probability of obtaining a test statistic at least as extreme as the observed data, given H_0 is true.

So the p-value is the probability of rejecting H_0 with the value of the test statistic obtained from the data given H_0 is true. That is, it is the critical value of α with regards to the hypothesis test decision.

If we report the conclusion of the test, as well as the p value then the reader can decide how sensitive our result was to our choice of α.

Definition 19.4.2. **Coffee machine (continued).**
Compute the p value for the test in Example 19.3.1.

In Example 19.3.1 (Coffee machine), we were given $\bar{x} = 5.94$, $n = 20$ and $\sigma = 0.2$. Our decision rule was to reject H_0 if $|Z| = \left|\frac{\bar{x}-6.0}{0.2/\sqrt{20}}\right| > z_{0.025}$.

To compute the p-value for the test assume H_0 is true, that is, $\mu = 6.0$. We want to find,

$$\begin{aligned} P(\,|\bar{x}-\mu| > |5.94-\mu|\,) &= P\left(|Z| = \left|\frac{\bar{x}-6.0}{0.2/\sqrt{20}}\right| > \left|\frac{5.94-6.0}{0.2/\sqrt{20}}\right|\right) \\ &= P(|Z| > 1.34) \\ &= 2P(Z > 1.34) \\ &= 2 \times 0.0901 \\ &= 0.1802. \end{aligned}$$

Consider the following remarks on Example 19.4.2.

- The multiplication factor of 2 has arisen since we are computing the p value for a two-sided test, so there is an equal-sized rejection region at both tails of the distribution. For a one-tailed test we only need to compute the probability of rejecting in one direction.

- The p value implies that if we had chosen an α of at least 0.1802 then we would have been able to reject H_0.

- In applied statistics, the p value is interpreted as the sample providing:

$$\begin{cases} \text{strong evidence against } H_0, & \text{if } p \leq 0.01, \\ \text{evidence against } H_0, & \text{if } p \leq 0.05, \\ \text{slight evidence against } H_0, & \text{if } p \leq 0.10, \\ \text{no evidence against } H_0, & \text{if } p > 0.10. \end{cases}$$

19.5 Tests for normal means, σ unknown

Assume $X_1, X_2, \ldots, X_n$ is a random sample from a normal distribution with unknown variance σ^2.

Test 4: $H_0 : \mu = \mu_0$ vs. $H_1 : \mu < \mu_0$; σ^2 unknown.

As before the decision rule is to reject H_0 if $\bar{X} < c$ for some cut off value c that we need to find. We have

$$\begin{aligned} \alpha &= P(\text{Type I error}) \\ &= P(\text{Reject } H_0 | H_0 \text{ true}) \\ &= P(\bar{X} < c | \mu = \mu_0) \\ &= P\left(\bar{X} < c | \bar{X} \sim N\left(\mu_0, \frac{\sigma^2}{n}\right)\right). \end{aligned}$$

However, now σ^2 is unknown. We have seen before that

$$\frac{\bar{X} - \mu_0}{s/\sqrt{n}} \sim t_{n-1},$$

where s^2 is the sample variance.

Hence,

$$\begin{aligned}\alpha &= P\left(\bar{X} < c | \bar{X} \sim N\left(\mu_0, \frac{\sigma^2}{n}\right)\right) \\ &= P\left(\frac{\bar{X}-\mu_0}{s/\sqrt{n}} < \frac{c-\mu_0}{s/\sqrt{n}}\right) \\ &= P\left(T < \frac{c-\mu_0}{s/\sqrt{n}}\right).\end{aligned}$$

Now, $P(T < -t_{n-1,\alpha}) = \alpha$, where $t_{n-1,\alpha}$ can be found by using the `qt` function in **R** with $t_{n-1,\alpha}$ = `qt(alpha,n-1)` or using statistical tables similar to those of the normal tables in Section 5.7. Therefore

$$-t_{n-1,\alpha} = \frac{c-\mu_0}{s/\sqrt{n}}$$

and $c = \mu_0 - t_{n-1,\alpha} \cdot \frac{s}{\sqrt{n}}$. Therefore, the **decision rule** is to reject H_0 if $\bar{X} < \mu_0 - t_{n-1,\alpha} \cdot \frac{s}{\sqrt{n}}$ or, equivalently if

$$T = \frac{\bar{X}-\mu_0}{s/\sqrt{n}} < -t_{n-1,\alpha}.$$

Test 5: $H_0 : \mu = \mu_0$ vs. $H_1 : \mu > \mu_0$; σ^2 unknown.

This is similar to Test 4, except the **decision rule** is to reject H_0 if $\bar{X} > \mu_0 + t_{n-1,\alpha} \cdot \frac{s}{\sqrt{n}}$ or, equivalently if

$$T = \frac{\bar{X}-\mu_0}{s/\sqrt{n}} > t_{n-1,\alpha}.$$

Test 6: $H_0 : \mu = \mu_0$ vs. $H_1 : \mu \neq \mu_0$; σ^2 unknown.

Similarly deduced to Test 3, the **decision rule** here is to reject H_0 if

$$|T| = \left|\frac{\bar{X}-\mu_0}{s/\sqrt{n}}\right| > t_{n-1,\alpha/2}.$$

Example 19.5.1. **Coffee machine (continued).**
Suppose that σ is unknown in Example 19.3.1, though we still assume the amount of coffee dispensed is normally distributed. A random sample of $n = 20$ cups gives mean $\bar{x} = 5.94$ and sample standard deviation $s = 0.1501$.
Test whether the machine is correctly filling the cups.

We test $H_0 : \mu = 6.0$ vs. $H_1 : \mu \neq 6.0$ at significance level $\alpha = 0.05$.

The decision rule is to reject H_0 if $|T| = \left|\frac{\bar{x}-6.0}{0.1501/\sqrt{20}}\right| > t_{20-1,0.05/2} = t_{19,0.025} = 2.093$.

Now

$$|T| = \left|\frac{5.94 - 6.0}{0.1501/\sqrt{20}}\right| = |-1.7876| < 2.093.$$

Therefore, we do not reject H_0 at $\alpha = 0.05$. The p value is

$$\begin{aligned} p &= P(|\bar{x} - 6.0| > |5.94 - 6.0|) \\ &= 2P(t_{19} > |-1.7876|) \\ &= 2 \times 0.0449 \\ &= 0.0898. \end{aligned}$$

19.6 Confidence intervals and two-sided tests

Consider the two-sided t-test of size α. We reject H_0 if $|T| = \left|\frac{\bar{X}-\mu_0}{s/\sqrt{n}}\right| > t_{n-1,\alpha/2}$. This implies we do not reject H_0 if

$$|T| = \left|\frac{\bar{X} - \mu_0}{s/\sqrt{n}}\right| \leq t_{n-1,\alpha/2}$$

or equivalently,

$$\begin{aligned} -t_{n-1,\alpha/2} \cdot \tfrac{s}{\sqrt{n}} \leq \bar{X} - \mu_0 \leq t_{n-1,\alpha/2} \cdot \tfrac{s}{\sqrt{n}} \\ \bar{X} - t_{n-1,\alpha/2} \cdot \tfrac{s}{\sqrt{n}} \leq \mu_0 \leq \bar{X} + t_{n-1,\alpha/2} \cdot \tfrac{s}{\sqrt{n}}. \end{aligned}$$

But

$$\left(\bar{X} - t_{n-1,\alpha/2}\frac{s}{\sqrt{n}}, \bar{X} + t_{n-1,\alpha/2}\frac{s}{\sqrt{n}}\right)$$

is a $100(1-\alpha)\%$ confidence interval for μ. Consequently, if μ_0, the value of μ under H_0, falls within the $100(1-\alpha)\%$ confidence interval for μ, then we will **not** reject H_0 at significance level α.

In general, therefore, there is a correspondence between the "acceptance region" of a statistical test of size α and the related $100(1-\alpha)\%$ confidence interval. Therefore, we will **not** reject $H_0 : \theta = \theta_0$ vs. $H_1 : \theta \neq \theta_0$ at level α if and only if θ_0 lies within the $100(1-\alpha)\%$ confidence interval for θ.

Definition 19.6.1. **Coffee machine (continued).**
For the coffee machine in Example 19.5.1 (Coffee machine - continued) we wanted to test $H_0 : \mu = 6.0$ vs. $H_1 : \mu \neq 6.0$ at significance level $\alpha = 0.05$. We were given a random sample of $n = 20$ cups with $\bar{x} = 5.94$ and $s^2 = 0.1501^2$. Construct a 95% confidence interval for μ.

The limits of a 95% confidence interval for μ are

$$\begin{aligned} \bar{x} \pm t_{n-1,\alpha/2}\frac{s}{\sqrt{n}} &= 5.94 \pm t_{20-1,0.05/2}\frac{0.1501}{\sqrt{20}} \\ &= 5.94 \pm 2.093\frac{0.1501}{\sqrt{20}} \end{aligned}$$

so the 95% confidence interval for μ is

$$(5.8698, 6.0102).$$

If we use the confidence interval to perform our test, we see that

$$\mu_0 = 6.0 \in (5.8698, 6.0102),$$

so we will not reject H_0 at $\alpha = 0.05$.

19.7 Distribution of the variance

Thus far we have considered hypothesis testing for the mean but we can also perform hypothesis tests for the variance of a normal distribution. However, first we need to consider the distribution of the sample variance.

Suppose that $Z_1, Z_2, \ldots, Z_n \sim N(0,1)$. Then we have shown that

$$Z_1^2 \sim \chi_1^2 = \text{Gamma}\left(\frac{1}{2}, \frac{1}{2}\right),$$

in Section 14.2.

This can be extended to show that

$$\sum_{i=1}^{n} Z_i^2 \sim \chi_n^2 = \text{Gamma}\left(\frac{n}{2}, \frac{1}{2}\right).$$

More generally, if $X_1, X_2, \ldots, X_n \sim N(\mu, \sigma^2) = \mu + \sigma Z$, then

$$\frac{1}{\sigma^2} \sum_{i=1}^{n} \left(X_i - \bar{X}\right)^2 \sim \chi_{n-1}^2.$$

Note that the *degrees of freedom* of χ^2 is $n-1$, the number of observations n minus 1 for the estimation of μ by $\bar{X}$.

It follows that

$$(n-1)\frac{s^2}{\sigma^2} \sim \chi_{n-1}^2.$$

19.8 Other types of tests

Test 7: $H_0 : \sigma_1^2 = \sigma_2^2$ vs. $H_1 : \sigma_1^2 \neq \sigma_2^2$.

Let $X_1, X_2, \ldots, X_m \sim N(\mu_1, \sigma_1^2)$ and $Y_1, Y_2, \ldots, Y_n \sim N(\mu_2, \sigma_2^2)$ be two independent random samples from normal populations.

The test statistic is $F = \frac{s_1^2}{s_2^2}$, where

$$s_1^2 = \frac{1}{m-1} \sum_{i=1}^{m} (X_i - \bar{X})^2, \qquad \text{and} \qquad s_2^2 = \frac{1}{n-1} \sum_{i-1}^{n} (Y_i - \bar{Y})^2.$$

Recall that

$$(m-1)\frac{s_1^2}{\sigma_1^2} \sim \chi_{m-1}^2, \qquad \text{and} \qquad (n-1)\frac{s_2^2}{\sigma_2^2} \sim \chi_{n-1}^2.$$

Since the samples are independent, s_1^2 and s_2^2 are independent. Therefore,

$$\frac{s_1^2/\sigma_1^2}{s_2^2/\sigma_2^2} \sim \frac{\chi_{m-1}^2/(m-1)}{\chi_{n-1}^2/(n-1)} \sim F_{m-1,n-1}.$$

Under $H_0 : \sigma_1^2 = \sigma_2^2$, it follows

$$F = \frac{s_1^2}{s_2^2} \sim F_{m-1,n-1}.$$

The **decision rule** is to reject H_0 if

$$F = \frac{s_1^2}{s_2^2} < F_{m-1,n-1,\alpha/2}, \qquad \text{or} \qquad F = \frac{s_1^2}{s_2^2} > F_{m-1,n-1,1-\alpha/2}.$$

The critical values $F_{m-1,n-1,\alpha/2}$ and $F_{m-1,n-1,1-\alpha/2}$ are given using `qf(alpha/2,m-1,n-1)` and `qf(1-alpha/2,m-1,n-1)`. Alternatively, Statistical Tables can be used. For the latter you may need to use the identity

$$F_{\nu_1,\nu_2,q} = \frac{1}{F_{\nu_2,\nu_1,1-q}},$$

to obtain the required values from the table.

Test 8: $H_0 : \mu_1 = \mu_2$ vs. $H_1 : \mu_1 \neq \mu_2$; σ^2 unknown.

Assume $X_1, X_2, \ldots, X_m \sim N(\mu_1, \sigma^2)$ and $Y_1, Y_2, \ldots, Y_n \sim N(\mu_2, \sigma^2)$ are two independent random samples with unknown but equal variance σ^2.

Note that

- $(\bar{X} - \bar{Y}) \sim N\Big((\mu_1 - \mu_2), \sigma^2 \left(\frac{1}{m} + \frac{1}{n}\right)\Big)$ which implies
$$\frac{(\bar{X} - \bar{Y}) - (\mu_1 - \mu_2)}{\sqrt{\sigma^2 \left(\frac{1}{m} + \frac{1}{n}\right)}} \sim N(0, 1);$$
- $(m + n - 2)\frac{s_p^2}{\sigma^2} \sim \chi^2_{m+n-2}$;
- s_p^2 is independent of $\bar{X} - \bar{Y}$.

Therefore,

$$\frac{(\bar{X} - \bar{Y}) - (\mu_1 - \mu_2)}{\sqrt{s_p^2 \left(\frac{1}{m} + \frac{1}{n}\right)}} = \frac{\frac{(\bar{X}-\bar{Y})-(\mu_1-\mu_2)}{\sqrt{\sigma^2(\frac{1}{m}+\frac{1}{n})}}}{\sqrt{\frac{(m+n-2)s_p^2}{(m+n-2)\sigma^2}}} \sim t_{m+n-2}.$$

Under H_0, $\mu_1 - \mu_2 = 0$, this becomes

$$T = \frac{\bar{X} - \bar{Y}}{\sqrt{s_p^2\left(\frac{1}{m} + \frac{1}{n}\right)}} \sim t_{m+n-2}.$$

Therefore the **decision rule** is to reject H_0 if

$$|T| = \left|\frac{\bar{X} - \bar{Y}}{\sqrt{s_p^2\left(\frac{1}{m} + \frac{1}{n}\right)}}\right| > t_{m+n-2,\alpha/2},$$

where $s_p^2 = \frac{(m-1)s_X^2 + (n-1)s_Y^2}{m+n-2}$ is the pooled sample variance.

Example 19.8.1. **Blood bank.**
Suppose that one wants to test whether the time it takes to get from a blood bank to a hospital via two different routes is the same on average. Independent random samples are selected from each of the different routes and we obtain the following information:

Route X	$m = 10$	$\bar{x} = 34$	$s_X^2 = 17.111$
Route Y	$n = 12$	$\bar{y} = 30$	$s_Y^2 = 9.454$

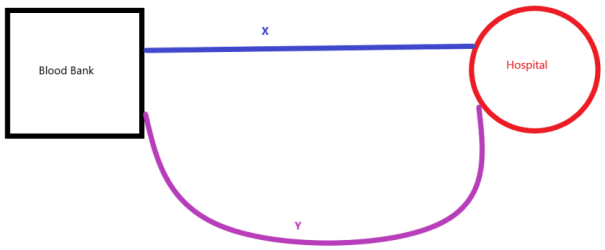


Figure 19.1: Routes from blood bank to hospital.

Test $H_0 : \mu_X = \mu_Y$ vs. $H_1 : \mu_X \neq \mu_Y$ at significance level $\alpha = 0.05$, where μ_1 and μ_2 denote the mean travel times on routes X and Y, respectively.

Attempt Example 19.8.1: Blood bank and then watch Video 29 for the solutions.

Watch Video 29: Blood bank

Solution to Example 19.8.1: Blood bank

To perform the t-test we need the variances to be equal, so we test $H_0 : \sigma_X^2 = \sigma_Y^2$ vs. $H_1 : \sigma_X^2 \neq \sigma_Y^2$ at significance level $\alpha = 0.05$. The decision rule is to reject

H_0 if

$$F = \frac{s_X^2}{s_Y^2} < F_{m-1,n-1,\alpha/2} \qquad \text{or} \qquad F = \frac{s_X^2}{s_Y^2} > F_{m-1,n-1,1-\alpha/2}.$$

Compute

- $F = \frac{s_X^2}{s_Y^2} = \frac{17.111}{9.454} = 1.81$;
- $F_{9,11,0.975} = \frac{1}{F_{11,9,0.025}} = \frac{1}{3.915} = 0.256$;
- $F_{9,11,0.025} = 3.588$.

Hence $F_{9,11,0.975} < F < F_{9,11,0.025}$, so we do not reject H_0 at $\alpha = 0.05$. Therefore we can assume the variances from the two samples are the same.

Now we test $H_0 : \mu_X = \mu_Y$ vs. $H_1 : \mu_X \neq \mu_Y$ at significance level $\alpha = 0.05$

The decision rule is to reject H_0 if

$$|T| = \left| \frac{\bar{X} - \bar{Y}}{\sqrt{s_p^2 \left(\frac{1}{m} + \frac{1}{n}\right)}} \right| > t_{m+n-2,\alpha/2}.$$

Computing, the pooled variance,

$$s_p^2 = \frac{9 \times 17.111 + 11 \times 9.454}{10 + 12 - 2} = 12.9$$

giving

$$T = \left| \frac{34 - 30}{\sqrt{12.9 \left(\frac{1}{10} + \frac{1}{12}\right)}} \right| = 2.601 > t_{20,0.025} = 2.086.$$

Therefore we reject H_0 that the journey times are the same on average at $\alpha = 0.05$. The p value is

$$P(|T| > 2.601) = 2P(T > 2.601) = 2 \times 0.00854 = 0.01708.$$

Test 9: $H_0 : \mu_1 = \mu_2$ vs. $H_1 : \mu_1 \neq \mu_2$; non-independent samples.

Suppose that we have two groups of observations $X_1, X_2, \ldots, X_n$ and $Y_1, Y_2, \ldots, Y_n$ where there is an obvious pairing between the observations. For example consider before and after studies or comparing different measuring devices. This means the samples are no longer independent.

An equivalent hypothesis test to the one stated is $H_0 : \mu_d = \mu_1 - \mu_2 = 0$ vs. $H_1 : \mu_d = \mu_1 - \mu_2 \neq 0$. With this in mind define $D_i = X_i - Y_i$ for $i = 1, \ldots, n$, and assume $D_1, D_2, \ldots, D_n \sim N(\mu_d, \sigma_d^2)$ and are i.i.d.

The **decision rule** is to reject H_0 if

$$\left| \frac{\bar{D}}{s_d/\sqrt{n}} \right| > t_{n-1,\alpha/2}.$$

Example 19.8.2. **Drug Trial.**
In a medical study of patients given a drug and a placebo, sixteen patients were paired up with members of each pair having a similar age and being the same sex. One of each pair received the drug and the other recieved the placebo. The response score for each patient was found.

Pair Number	1	2	3	4	5	6	7	8
Given Drug	0.16	0.97	1.57	0.55	0.62	1.12	0.68	1.69
Given Placebo	0.11	0.13	0.77	1.19	0.46	0.41	0.40	1.28

Are the responses for the drug and placebo significantly different?

This is a "matched-pair" problem, since we expect a relation between the values of each pair. The difference within each pair is

Pair Number	1	2	3	4	5	6	7	8
$\mathbf{D_i = y_i - x_i}$	0.05	0.84	0.80	−0.64	0.16	0.71	0.28	0.41

We consider the D_i's to be a random sample from $N(\mu_D, \sigma_D^2)$. We can calculate that $\bar{D} = 0.326$, $s_D^2 = 0.24$ so $s_D = 0.49$.

To test $H_0 : \mu_D = 0$ vs $H_1 : \mu_D \neq 0$, the decision rule is to reject H_0 if

$$\left|\frac{\bar{D}}{s_D/\sqrt{n}}\right| = 1.882 > t_{n-1,\alpha/2}.$$

Now $t_{7,0.05} = 1.895$, so we would not reject H_0 at the 10% level (just).

19.9 Sample size calculation

We have noted that for a given sample $x_1, x_2, \ldots, x_n$, if we decrease the Type I error α then we increase the Type II error β, and visa-versa.

To control for both Type I and Type II error, ensure that α and β are both sufficiently small, we need to choose an appropriate sample size n.

Sample size calculations are appropriate when we have two simple hypotheses to compare. For example, we have a random variable X with unknown mean $\mu = E[X]$ and known variance $\sigma^2 = \text{Var}(X)$. We compare the hypotheses:

- $H_0 : \mu = \mu_0$,
- $H_1 : \mu = \mu_1$.

Without loss of generality we will assume that $\mu_0 < \mu_1$.

Suppose that $x_1, x_2, \ldots, x_n$ represent i.i.d. samples from X. Then by the central limit theorem

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i \approx N\left(\mu, \frac{\sigma^2}{n}\right).$$

We reject H_0 at an α significance level if

$$\frac{\bar{x} - \mu_0}{\sigma/\sqrt{n}} > z_\alpha.$$

That is, we reject the null hypothesis $\mu = \mu_0$ in favour of the alternative hypothesis $\mu = \mu_1$ if

$$\bar{x} > \mu_0 + z_\alpha \frac{\sigma}{\sqrt{n}}.$$

Note that as n increases, the cut-off for rejecting H_0 decreases towards μ_0.

We now consider the choice of n to ensure that the Type II error is at most β, or equivalently, that the power of the test is at least $1 - \beta$.

The Power of the test is:

$$\text{Power} = \text{P}(\text{Reject } H_0 | H_0 \text{ is false}).$$

Rewriting in terms of the test statistic and H_0 is false (H_1 is true):

$$\begin{aligned} \text{Power} &= \text{P}\left(\frac{\bar{X} - \mu_0}{\sigma/\sqrt{n}} > z_\alpha \middle| \mu = \mu_1 \right) \\ &= 1 - \beta. \end{aligned}$$

Lemma 19.9.1 (Sample size calculation) gives the smallest sample size n to bound Type I and II errors by α and β in the case where the variance, σ^2 is known.

Lemma 19.9.1. **Sample size calculation.**
Suppose that X is a random variable with unknown mean μ and known variance σ^2. The required sample size, n, to ensure significance level α and power $1 - \beta$ for comparing hypotheses:

- $H_0 : \mu = \mu_0$
- $H_1 : \mu = \mu_1$

is:

$$n = \left(\frac{\sigma}{\mu_1 - \mu_0} (z_\alpha - z_{1-\beta}) \right)^2.$$

The details of the proof of Lemma 19.9.1 (Sample size calculation) are provided but can be omitted.

Proof of Sample Size calculations.

Thus the Power of the test is:

$$\begin{aligned} \text{Power} = 1 - \beta &= \text{P}\left(\frac{\bar{X} - \mu_1 + \mu_1 - \mu_0}{\sigma/\sqrt{n}} > z_{1-\alpha} \middle| \mu = \mu_1 \right) \\ &= \text{P}\left(\frac{\bar{X} - \mu_1}{\sigma/\sqrt{n}} + \frac{\mu_1 - \mu_0}{\sigma/\sqrt{n}} > z_{1-\alpha} \middle| \mu = \mu_1 \right) \\ &= \text{P}\left(\frac{\bar{X} - \mu_1}{\sigma/\sqrt{n}} > z_{1-\alpha} - \frac{\mu_1 - \mu_0}{\sigma/\sqrt{n}} \middle| \mu = \mu_1 \right). \end{aligned}$$

Given $\mu = \mu_1$, we have that:

$$\frac{\bar{X}-\mu_1}{\sigma/\sqrt{n}} \sim Z = N(0,1).$$

Therefore the power satisfies:

$$\begin{aligned} \mathrm{P}\left(Z > z_\alpha - \frac{\mu_1-\mu_0}{\sigma/\sqrt{n}} \middle| \mu = \mu_1\right) &= 1-\beta \\ &= P(Z > z_{1-\beta}). \end{aligned}$$

Hence,

$$z_\alpha - \frac{\mu_1-\mu_0}{\sigma/\sqrt{n}} = z_{1-\beta},$$

which rearranges to give

$$n = \left(\frac{\sigma}{\mu_1-\mu_0}(z_\alpha - z_{1-\beta})\right)^2.$$

Note:

1. We need larger n as σ increases. (More variability in the observations.)

2. We need larger n as $\mu_1-\mu_0$ gets closer to 0. (Harder to detect a small difference in mean.)

3. We have that $\alpha, \beta < 0.5$, so $z_\alpha > 0$ and $z_{1-\beta} < 0$. Hence, $z_\alpha - z_{1-\beta}$ becomes larger as α and β decrease. (Smaller errors requires larger n.)

The following R Shiny App lets you explore the effect of $\mu_1-\mu_0$, σ and α on the sample size n or power $1-\beta$.

R Shiny app: Sample size calculation app

Task: Session 10

Attempt the **R Markdown** file for Session 10:
Session 10: Confidence intervals and hypothesis testing

Student Exercises

Attempt the exercises below.

Note that throughout the exercises, for a random variable X and $0 < \beta < 1$, c_β satisfies $\mathrm{P}(X > c_\beta) = \beta$.

Exercise 19.1.
Eleven bags of sugar, each nominally containing 1 kg, were randomly selected from a large batch. The weights of sugar were:

$$1.02,\ 1.05,\ 1.08,\ 1.03,\ 1.00,\ 1.06,\ 1.08,\ 1.01,\ 1.04,\ 1.07,\ 1.00.$$

You may assume these values are from a normal distribution.

(a) Calculate a 95% confidence interval for the mean weight for the batch.

(b) Test the hypothesis $H_0 : \mu = 1$ vs $H_1 : \mu \neq 1$. Give your answer in terms of a p-value.

Note that

β	0.1	0.05	0.025	0.01	0.005	0.001	0.0005	0.0001
$t_{10} : c_\beta$	1.3722	1.8125	2.2281	2.7638	3.1693	4.1437	4.5869	5.6938
$Z : c_\beta$	1.2816	1.6449	1.96	2.3263	2.5758	3.0902	3.2905	3.719

Exercise 19.2.
Random samples of 13 and 11 chicks, respectively, were given from birth a protein supplement, either oil meal or meat meal. The weights of the chicks when six weeks old are recorded and the following sample statistics obtained:

$$\begin{array}{lccc} \text{Oil Meal Data:} & \bar{x}_1 = 247.9 & s_1^2 = 2925.8 & n_1 = 13 \\ \text{Meat Meal Data:} & \bar{x}_2 = 275.5 & s_2^2 = 4087.3 & n_2 = 11 \end{array}$$

(a) Carry out an F-test to examine whether or not the groups have significantly different variances or not.

(b) Calculate a 95% confidence interval for the difference between weights of 6-week-old chicks on the two diet supplements.

(c) Do you consider that the supplements have a significantly different effect? Justify your answer.

Note that

$F_{10,12}$:

β	0.05	0.025	0.01	0.005
c_β	2.7534	3.3736	4.2961	5.0855

$F_{12,10}$:

β	0.05	0.025	0.01	0.005
c_β	2.913	3.6209	4.7059	5.6613

.

β	0.1	0.05	0.025	0.01	0.005	0.001	0.0005	0.0001
$t_{22} : c_\beta$	1.3212	1.7171	2.0739	2.5083	2.8188	3.505	3.7921	4.452

Exercise 19.3.
A random sample of 12 car drivers took part in an experiment to find out if alcohol increases the average reaction time. Each driver's reaction time was measured in a laboratory before and after drinking a specified amount of alcoholic beverage. The reaction times were as follows:

	1	2	3	4	5	6	7	8	9	10	11	12
Before	0.68	0.64	0.82	0.8	0.72	0.55	0.84	0.78	0.57	0.73	0.86	0.74
After	0.73	0.62	0.92	0.87	0.77	0.7	0.88	0.78	0.66	0.79	0.86	0.72

Let μ_B and μ_A be the population mean reaction time, before and after drinking alcohol.

(a) Test $H_0 : \mu_B = \mu_A$ vs. $H_1 : \mu_B \neq \mu_A$ assuming the two samples are independent.

(b) Test $H_0 : \mu_B = \mu_A$ vs. $H_1 : \mu_B \neq \mu_A$ assuming the two samples contain 'matched pairs'.

(c) Which of the tests in (a) and (b) is more appropriate for these data, and why?

Note that

β	0.1	0.05	0.025	0.01	0.005	0.001	0.0005	0.0001
$t_{11} : c_\beta$	1.3634	1.7959	2.201	2.7181	3.1058	4.0247	4.437	5.4528

and the critical values for t_{22} are given above in Exercise 19.2.

Chapter 20

Hypothesis Testing Discrete Data

20.1 Introduction

In Section 19 (Hypothesis Testing) we have studied hypothesis testing for normal random variables and through the central limit theorem sums (and means) of random variables. The normal distribution is a continuous distribution and there are many situations where we want to compare hypotheses with data or distributions which are discrete. These include:-

- Fitting a discrete probability distribution to data. Goodness-of-fit
- Testing independence between two discrete variables (contingency tables).

20.2 Goodness-of-fit motivating example

We start with a motivating example.

Example 20.2.1. **Film stars.**
A film studio wants to decide which actor or actress to hire for the main role in a series of movies.

They have a shortlist of 5 and decide to ask the public who their favourite actor or actress is.

1,000 people are randomly selected and asked who their favourite actor or actress is from the shortlist of 5.

Results:

Preferred Actor	1	2	3	4	5

Preferred Actor	1	2	3	4	5
Frequency	225	189	201	214	171

An investor in the film claims "There is no difference in who the public prefer we should hire the cheapest!"

Does the data support the investor's claim?

We work through testing the investor's claim via a series of steps.

Step 1
Interpret what the investor's claim represents statistically.

"No difference in who the public prefers" means that if we choose an individual at random from the population they are equally likely to choose each of the five actors/actresses. That is, probability 1/5 of each actor/actress being chosen.

Step 2
What would we **expect** to observe in the data if the investor's claim is true?

The investor's claim has led us to a **model** where each actor/actress has probability 1/5 of being selected by a member of the public. Therefore when 1000 people are asked, we would expect each actor/actress to receive:

$$1000 \times \frac{1}{5} = 200 \text{ votes.}$$

Thus based on the **model** of the investor's claim:

Preferred Actor	1	2	3	4	5
Frequency	225	189	201	214	171
Expected	200	200	200	200	200

Step 3
Is what we **observe** (Frequency) in the data consistent with what we **expect** (Expected) to see if the investor's claim is a good model?

In hypothesis testing language, should we reject or not the null hypothesis:

H_0: All actors equally popular.

In favour of the alternative hypothesis:

H_1: There is a difference in popularity between at least two actors.

To compare competing hypotheses we require a **test statistic** and a **sampling distribution** for the test statistic under the assumption that the null hypothesis is true.

Test Statistic

For each outcome (actor), let O_i and E_i denote the number of **observed** and **expected** votes for actor i.

The test statistic χ^2_{obs} is

$$\chi^2_{obs} = \sum_i \frac{(O_i - E_i)^2}{E_i}.$$

For the actors example,

$$\chi^2_{obs} = \frac{(225-200)^2}{200} + \frac{(189-200)^2}{200} + ... + \frac{(171-200)^2}{200} = 8.92.$$

Sampling distribution

We reject H_0 at a significance level α if

$$\chi^2_{obs} \geq \chi^2_{\nu,\alpha},$$

where $\chi^2_{\nu,\alpha}$ is the $(1-\alpha)100\%$ quantile of the χ^2 distribution with ν degrees of freedom and

$$\nu = \text{Number of categories} - 1 = 5 - 1 = 4.$$

Thus if X is a χ^2 distribution with ν degrees of freedom then

$$\mathrm{P}\left(X \leq \chi^2_{\nu,\alpha}\right) = 1 - \alpha$$

or equivalently,

$$\mathrm{P}\left(X > \chi^2_{\nu,\alpha}\right) = \alpha.$$

Since $\chi^2_{4,0.05} = 9.488$, we **do not reject** the null hypothesis at a 5% significance level. That is, the investor's claim of all actors being equally popular is reasonable given the observed data.

20.3 Goodness-of-fit

We describe the general procedure for testing the goodness-of-fit of a probability distribution to data using the χ-squared distribution.

Suppose that we have N independent observations, $y_1, y_2, \ldots, y_N$ from an unknown probability distribution, Y. Suppose that there are n categories covering the possible outcomes and for $i = 1, 2, \ldots, n$, let $\mathcal{C}_i$ denote category i. For example, we could have $\mathcal{C}_i = \{y = i\}$, the observations equal to i, or $\mathcal{C}_i = \{a_i < y \leq b_i\}$, the observations equal in the range $(a_i, b_i]$.

For $i = 1, 2, \ldots, n$, let

$$O_i = \#\{y_j \in \mathcal{C}_i\},$$

the number of data points **observed** in category i.

We propose a probability distribution X for the unknown probability distribution, Y. This gives us our null hypothesis:

H_0: $Y = X$

with the alternative hypothesis

H_1: $Y \neq X$.

Under the null hypothesis, we calculate for each category i, the **expected** number of observations we would expect to belong to category i. That is, for $i = 1, 2, \ldots, n$,

$$E_i = N \times \mathrm{P}(X \in \mathcal{C}_i).$$

We compute the test statistic χ^2_{obs} is

$$\chi^2_{obs} = \sum_i \frac{(O_i - E_i)^2}{E_i},$$

and the number of degrees of freedom, $\nu = n - 1$.

We choose a significance level α and reject the null hypothesis at the significance level if

$$\chi^2_{obs} > \chi^2_{\nu, 1-\alpha}.$$

Important points

1. The test statistic, under the null hypothesis, does *not exactly* follow a χ^2 distribution. As with the central limit theorem, the test statistic is approximately χ^2 distributed with the approximation becoming better as the amount of data in each category increases.

2. For discrete data it will often be natural to choose $\mathcal{C}_i = \{y = i\}$, whereas for continuous data we have considerable flexibility in choosing the number of categories and the category intervals. The considerations on choice of categories for goodness-of-fit testing are not dissimilar to the considerations on choice of bins for histograms.

3. The expected frequencies in each category should not be too small with a rule of thumb that $E_i \geq 5$. If some of the expected frequencies are less than 5 then we pool categories such that the expected frequency of the two (or more) categories combined is greater than or equal to 5.

4. We will often want to fit a probability distribution X from a given family of probability distributions (*e.g.* Poisson, Gamma) without necessarily *a priori* choosing the parameters of the distribution. For example, we might choose to fit a Poisson distribution with mean λ to a data set and use the sample mean, $\bar{y}$, as the choice of λ. The goodness-of-fit procedure is as above except that we reduce the number of degrees of freedom by 1 for each parameter we estimate from the data,

$$\nu = \#\text{Categories} - 1 - \#\text{Estimated Parameters}.$$

Example 20.3.1. **Alleles.**
Each person is one of the following genotypes A/A, A/S or S/S.

The observed frequencies in a population of $N = 886$ are:

$$A/A : 700, \qquad A/S : 180, \qquad S/S : 6$$

Hypothesis:
The proportion of people with each genotype is

$$p^2,\ 2p(1-p) \text{ and } (1-p)^2,$$

where p is the proportion of alleles that are of type A.

Is this a reasonable model for the data?

Watch Video 30 for the worked solutions to Example 20.3.1 (Alleles)

Watch Video 30: Alleles

Solution to Example 20.3.1: Alleles.

We start with finding a suitable choice for p.

We can estimate by p by $\hat{p}$ the proportion of alleles of type A in the population:

$$\hat{p} = \frac{2 \times 700 + 180}{2 \times 886} = 0.8916.$$

This is the MLE for p.

Therefore the probabilities for each genotype are:

$$\begin{aligned} \mathrm{P}(A/A) &= p^2 = 0.8916479^2 = 0.795 \\ \mathrm{P}(A/S) &= 2p(1-p) = 2 \times 0.8916479 \times (1 - 0.8916479) = 0.1932 \\ \mathrm{P}(S/S) &= (1-p)^2 = (1 - 0.8916479)^2 = 0.0117. \end{aligned}$$

Multiply the probabilities by $N = 886$ to give the **expected** numbers for each genotype:

$$\begin{aligned} A/A : N\mathrm{P}(A/A) &= 886 \times 0.795 = 704.4 \\ A/S : N\mathrm{P}(A/S) &= 886 \times 0.1932 = 171.2 \\ S/S : N\mathrm{P}(S/S) &= 886 \times 0.0117 = 10.4. \end{aligned}$$

The test statistics is

$$\begin{aligned} \chi^2_{obs} &= \sum_i \frac{(O_i - E_i)^2}{E_i} \\ &= \frac{(700 - 704.4)^2}{704.4} + \frac{(180 - 171.2)^2}{171.2} + \frac{(6 - 10.4)^2}{10.4} \\ &= 0.0275 + 0.4523 + 1.8615 = 2.3413. \end{aligned}$$

Since we have $n = 3$ categories and estimated 1 parameter (p), we have that the degrees of freedom is:

$$\nu = 3 - 1 - 1 = 1.$$

At 0.05% significance level: $\chi^2_{1,0.05} = 3.8415$.

Since, $\chi^2_{obs} < \chi^2_{1,0.05}$, there is no evidence to reject the null hypothesis.

The p-value is 0.126 (=P($W > \chi^2_{obs}$)), where W is a χ-square distribution with $\nu = 1$.

20.4 Testing Independence

Suppose that we have two categorical variables, A and B, where A can take m_A possible values and B can take m_B possible values.

Suppose that we have N observations with each observation belonging to one of the m_A categories of variable A and one of the m_B categories of variable B. For $i = 1, 2, \ldots, m_A$ and $j = 1, 2, \ldots, m_B$, let O_{ij} denote the number of observations which belong to category i of variable A **and** category j of variable B.

For example, variable A could be hair colour with categories:
1 - Brown
2 - Black
3 - Blonde
and variable B could be eye colour with categories:
1 - Brown
2 - Blue
3 - Green

Then N will be the total number of observations and O_{32} will be the number of observations (people) with Blonde hair and Blue eyes.

We often want to test the null hypothesis that the variables A and B are independent. For example, in the above scenario, the hypothesis that hair colour and eye colour are independent.

What does independence look like?

Let $p_{i\cdot}$ denote the probability that an individual in the population will belong to category i of variable A and let $p_{\cdot j}$ denote the probability that an individual in the population will belong to category j of variable B. Then if variables A and B are **independent**, the probability of individual belonging **both** to category i of variable A and category j of variable B is

$$p_{i\cdot} \times p_{\cdot j}.$$

Let

$$N_{i\cdot} = \sum_{j=1}^{m_B} O_{ij}$$

denote the total number of observations with variable A in category i and similarly let

$$N_{\cdot j} = \sum_{i=1}^{m_A} O_{ij}$$

denote the total number of observations with variable B in category j.

We can estimate $p_{i\cdot}$ by

$$\hat{p}_{i\cdot} = \frac{N_{i\cdot}}{N}$$

and $p_{\cdot j}$ by

$$\hat{p}_{\cdot j} = \frac{N_{\cdot j}}{N}.$$

This will give an estimate of

$$\hat{p}_{i\cdot} \times \hat{p}_{\cdot j} = \frac{N_{i\cdot}}{N} \times \frac{N_{\cdot j}}{N} = \frac{N_{i\cdot} N_{\cdot j}}{N^2}$$

for the probability of an individual belonging **both** to category i of variable A and category j of variable B under the null hypothesis of independence between variables A and B.

Therefore under the null hypothesis of independence the **expected** number of observations belonging to category i of variable A and category j of variable B is

$$E_{ij} = N \times \hat{p}_{i\cdot} \times \hat{p}_{\cdot j} = \frac{N_{i\cdot} N_{\cdot j}}{N}.$$

The test statistic χ^2_{obs} is again the sum of the square of the difference between the observed, O_{ij}, and the expected, E_{ij}, values divided by the expected values. That is,

$$\chi^2_{obs} = \sum_{i=1}^{m_A} \sum_{j=1}^{m_B} \frac{(O_{ij} - E_{ij})^2}{E_{ij}}.$$

The number of degrees of freedom is

$$\nu = (m_A - 1)(m_B - 1).$$

We reject the null hypothesis of independence between the variables A and B in favour of the alternative hypothesis that the variables A and B are dependent at a significance level α, if

$$\chi^2_{obs} > \chi^2_{\nu,\alpha}.$$

Example 20.4.1. **School children.**

A school take part in a study which involves recording the eye colour and hair colour of each child.

Observed		Eye		
		Brown	Blue	Green
Hair	Brown	117	14	21
	Black	56	3	11
	Blonde	17	41	19

The hypothesis which we wish to test is:

Are eye and hair colour independent?

The first step is to compute the row and column totals which give the total number of individuals with each hair colour and each eye colour, respectively.

		Eye			
		Brown	Blue	Green	Total
Hair	Brown	117	14	21	152
	Black	56	3	11	70
	Blonde	17	41	19	70
	Total	190	58	51	299

Then using $E_{ij} = N_{i\cdot}N_{\cdot j}/N$, we can compute the expected number of individuals in each category under the assumption of independence.

For example, the expected number of people with brown hair and brown eyes is

$$E_{11} = \frac{N_{i\cdot}N_{\cdot j}}{N} = \frac{152 \times 190}{299} = 96.6.$$

Therefore

Expected		Eye			
		Brown	Blue	Green	Total
Hair	Brown	96.6	29.5	25.9	152
	Black	44.5	13.6	11.9	70
	Blonde	48.9	14.9	13.2	77
	Total	190	58	51	299

.

We can the compute the differences between the observed and expected values. For example, for brown hair (hair category 1) and blue eyes (eye category 2), we have that:

$$\frac{(O_{12} - E_{12})^2}{E_{12}} = \frac{(14 - 29.5)^2}{29.5} = 8.14.$$

Therefore

$\frac{(O-E)^2}{E}$		Eye		
		Brown	Blue	Green
Hair	Brown	4.31	8.14	0.93
	Black	2.97	8.26	2.55
	Blonde	20.81	45.72	2.55

,

giving the test statistic to be

$$\chi^2_{obs} = \sum_{i=1}^{3}\sum_{j=1}^{3} \frac{(O_{ij} - E_{ij})^2}{E_{ij}} = 93.76.$$

Under the null hypothesis (independence), the test statistic approximately follow a χ^2 distribution with

$$\nu = (m_A - 1)(m_B - 1) = (3 - 1) \times (3 - 1) = 4$$

degrees of freedom.

Given that for a 0.1 significance level ($\alpha = 0.001$), the critical value for the χ^2 distribution is $\chi^2_{4,0.001} = 18.467$, there is very strong evidence to reject the null hypothesis. That is, there is very strong evidence that hair colour and eye colour are dependent.

Task: Session 11

Attempt the **R Markdown** file for Session 11:
Session 11: Goodness-of-fit

Student Exercises

Attempt the exercises below.

Exercise 20.1.
The following data give the frequency distribution of the size of casual groups of people on a spring afternoon in a park.

Size of Group	1	2	3	4	5	6
Frequency	1486	694	195	37	10	1

A suggested model for the probability p_r of a group of size r is

$$p_r = \frac{\mu^r \exp(-\mu)}{r![1 - \exp(-\mu)]}, \qquad r = 1, 2, \ldots,$$

where μ is estimated to be 0.89 for this data set.

Does this give a good fit to the data?

Exercise 20.2.
In order to test the lifetime of small batteries used to power clocks, 40 batteries were chosen at random and tested. Their times (in months) in failure were

18	11	25	36	40	72	33	51	1	12
46	28	87	75	24	11	23	13	45	2
40	79	14	59	1	7	39	54	16	3
8	2	52	20	9	6	7	26	31	38

The manufacturer claims that the lifetimes, X, have an exponential distribution with mean 30 months. If we assume this, calculate a, b, c and d such that

$$\begin{aligned}\frac{1}{5} &= P(0 < X < a) = P(a < X < b) = P(b < X < c) \\ &= P(c < X < d) = P(d < X < \infty).\end{aligned}$$

Construct a table of expected and observed frequencies for the above five intervals and hence test the manufacturer's claim by using a goodness-of-fit test at the 5% level.

Exercise 20.3.
In a clinical trial to test the effect of a new drug for influenza, 164 people with the condition were split into two equal groups, one of which was given the drug, the other a placebo. The table below indicates the response of the treatments.

	Helped	Harmed	No effect
Drug	50	10	22
Placebo	42	12	28

Test the hypothesis that the drug is no different from the placebo.

Chapter 21

Basic Hypothesis Tests for Linear Models

21.1 Introduction

In this section we consider the application of hypothesis testing to linear models. Suppose that we are given the linear model,

$$Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_{p-1} X_{(p-1)i} + \epsilon_i,$$

where $\epsilon_i \sim N(0, \sigma^2)$ are independent and identically distributed. We are interested in testing the hypothesis that a coefficient β_j is equal to some value b. In particular, we are most interested in $b = 0$ as setting $\beta_j = 0$ means that x_{ji} is not important in predicting Y_i, see Section 21.2. We can also construct confidence intervals for β_j and in Section 21.4 extend hypothesis testing to multiple (all) parameters to test whether or not a linear model is useful in a given modelling scenario.

21.2 Tests on a single parameter

Given the linear model,

$$Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_{p-1} X_{(p-1)i} + \epsilon_i,$$

where $\epsilon_i \sim N(0, \sigma^2)$, we want to test $H_0 : \beta_j = b$ vs. $H_1 : \beta_j \neq b$ at significance level α where b is some constant. Typically, we might choose $\alpha = 0.05$ (common

alternatives $\alpha = 0.01$ or $\alpha = 0.1$).

The **decision rule** is to reject H_0 if

$$|T| = \left| \frac{\hat{\beta}_j - b}{\text{SE}(\hat{\beta}_j)} \right| > t_{n-p,\alpha/2},$$

where $\text{SE}(\hat{\beta}_j) = \sqrt{\text{Var}(\hat{\beta}_j)}$ is the standard error of the parameter. Recall from Section 17 that $\text{Var}(\hat{\beta}_j) = s^2 \left((\mathbf{Z}^T \mathbf{Z})^{-1} \right)_{jj}$.

A special case of the above test occurs when we choose $b = 0$. The test $H_0 : \beta_j = 0$ vs. $H_1 : \beta_j \neq 0$ at level α has the **decision rule** to reject H_0 if

$$|T| = \left| \frac{\hat{\beta}_j}{\text{SE}(\hat{\beta}_j)} \right| > t_{n-p,\alpha/2}.$$

Note that if we reject $H_0 : \beta_j = 0$ we are claiming that the explanatory variable X_j is useful in predicting the response variable Y when all the other variables are included in the model.

The test statistic $|T| = \left| \frac{\hat{\beta}_j}{\text{SE}(\hat{\beta}_j)} \right|$ is often reported in the output from statistical software such as **R**.

Example 21.2.1. **Fuel consumption**
A dataset considers fuel consumption for 50 US states plus Washington DC, that is $n = 51$ observations. The response *fuel* is fuel consumption measured in gallons per person. The predictors considered are *dlic*, the percentage of licensed drivers, *tax*, motor fuel tax in US cents per gallon, *inc*, income per person in \$1,000s and *road*, the log of the number of miles of federal highway. Fitting a linear model of the form

$$\text{fuel} = \beta_0 + \beta_1 \cdot \text{dlic} + \beta_2 \cdot \text{tax} + \beta_3 \cdot \text{inc} + \beta_4 \cdot \text{road}$$

using **R**, the output is

	Estimate	Standard Error
β_0	154.19	194.906
β_1	4.719	1.285
β_2	-4.228	2.030
β_3	-6.135	2.194
β_4	26.755	9.337

Test $H_0 : \beta_2 = 0$ vs. $H_1 : \beta_2 \neq 0$ at significance level $\alpha = 0.05$.

Watch Video 31 for a work through in **R** of testing the null hypothesis.

Watch Video 31: Fuel consumption example

Hypothesis test for β_2.

The decision rule is to reject H_0 if

$$|T| = \left|\frac{\hat{\beta}_2}{\text{SE}(\hat{\beta}_2)}\right| = \left|\frac{-4.228}{2.030}\right| = |-2.083| > t_{46,0.025} = 2.013.$$

So we reject H_0 and conclude that the *tax* variable is useful for prediction of *fuel* after having included the other variables.

We note that the p-values is $P(|t_{46}| > 2.083) = 0.0428$ and therefore would not reject the null hypothesis $\beta_2 = 0$ at significance level $\alpha = 0.01$.

21.3 Confidence intervals for parameters

Recall that

$$|T| = \left|\frac{\hat{\beta}_j}{\text{SE}(\hat{\beta}_j)}\right| \sim t_{n-p}.$$

It follows that a $100(1-\alpha)\%$ confidence interval for β_j is

$$\left(\hat{\beta}_j - t_{n-p,\alpha/2}\text{SE}(\hat{\beta}_j), \hat{\beta}_j + t_{n-p,\alpha/2}\text{SE}(\hat{\beta}_j)\right)$$

where $\text{SE}(\hat{\beta}_j) = s\sqrt{((\mathbf{Z}^T\mathbf{Z})^{-1})_{jj}}$.

Example 21.3.1. **Fuel consumption (continued)**
Consider Example 21.2.1 (Fuel consumption), construct a 95% confidence interval for β_2.

A 95% confidence interval for β_2 is

$$\begin{aligned}
&\left(\hat{\beta}_2 - t_{46,0.025}\text{SE}(\hat{\beta}_j), \hat{\beta}_2 + t_{46,0.025}\text{SE}(\hat{\beta}_j)\right) \\
&= (-4.228 - 2.013 \times 2.030, -4.228 + 2.013 \times 2.030) \\
&= (-8.31, -0.14)
\end{aligned}$$

This confidence interval does not contain 0 (just) as we would expect from the calculation of the p-value in Example 20.2.1 (Fuel consumption) above.

21.4 Tests for the existence of regression

We want to test

$H_0 : \beta_1 = \beta_2 = \cdots = \beta_{p-1} = 0$

versus

$H_1 : \beta_j \neq 0$

for some j at significance level α.

Note that if we reject H_0 we are saying that the model

$$Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_{p-1} X_{(p-1)i}$$

has some ability to explain the variance that we are observing in Y. That is, there exists a linear relationship between the explanatory variables and the response variable.

If D_0 is the model deviance under the null hypothesis and D_1 is the model deviance under the alternative hypothesis, then the **decision rule** is to reject H_0 if

$$F = \frac{(D_0 - D_1)/(p-1)}{D_1/(n-p)} > F_{p-1,n-p,\alpha}.$$

Example 21.4.1. **Fuel consumption (continued)**
For the data in Example 21.2.1 (Fuel consumption), the two competing models are

$$M_1 : \text{fuel} = \beta_0 + \beta_1 \text{dlic} + \beta_2 \text{tax} + \beta_3 \text{inc} + \beta_4 \text{road}$$
$$M_0 : \text{fuel} = \beta_0$$

The models have residual sum of squares $D_1 = 193700$ and $D_0 = 395694.1$, respectively. We test $H_0 : \beta_1 = \cdots = \beta_4 = 0$ vs. $H_1 : \beta_j \neq 0$ for some $j = 1, \ldots, 4$ at level $\alpha = 0.05$.

The decision rule is to reject H_0 if

$$F = \frac{(395694.1 - 193700)/(5-1)}{193700/(51-5)} = \frac{50498.525}{4210.870} = 11.99 > F_{4,46,0.05} = 2.574.$$

Therefore, we reject H_0 and can say that the linear model has some power in explaining the variability in fuel.

Note that the p-value for the F test is $9.331 \times 10^{-7} = P(F_{4,46} > 11.99)$. This is given in **R** by `1-pf(11.99,4,46)` and is reported in the last line of `summary()` for a linear model in **R**.

Chapter 22

ANOVA Tables and F Tests

22.1 Introduction

In this section we will focus on the sources of variation in a linear model and how these can be used to determine the most appropriate linear model. We start in Section 22.2 by considering the residuals of the linear model and properties of the residuals. In Section 22.3, we introduce the total sum-of-squares **SStot** which is a measure of the total amount of variation in the model. This is comprised of two components: the regression sum-of-squares, **SSreg**, which measures the variability in the observations that is captured by the model and the residual sum-of-squares, **SSres**, which measures the unexplained variability in the observations. In Section 22.4, we introduce ANOVA tables for summarising variability in the model and testing null hypotheses. In particular, we consider the Fuel Consumption example, introduced in Section 21.2, and show how the conclusions obtained in Section 21.4 can be presented in the form of an ANOVA table. In Section 22.5, we consider two linear models for a given data set, where one model is *nested* within the other model. This allows us to compare two models which lie between the full model (includes all variables) and the null model (excludes all variables). Finally, in Section 22.6 we extend the comparison of nested models to sequential sum-of-squares to find the most appropriate model out of a range of nested linear models.

22.2 The residuals

Consider the linear model

$$\mathbf{y} = \mathbf{Z} \ + \ .$$

Recall the following model notation:

- $E[\ ] = \mathbf{0}$;
- Var( ) $= \sigma^2 \mathbf{I}_n$;
- $\hat{} = (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{y}$ is the *LSE* of ;
- $\hat{\mathbf{y}} = \mathbf{Z}\hat{}$ is the $n \times 1$ vector of *fitted values*;
- $\hat{\mathbf{y}} = \mathbf{P}\mathbf{y}$, where $\mathbf{P} = \mathbf{Z}(\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T$.

Let $\mathbf{r} = \hat{} = \mathbf{y} - \hat{\mathbf{y}}$ be the $n \times 1$ vector of *residuals*. Note that

$$\begin{aligned}\mathbf{r} &= \hat{} \\ &= \mathbf{y} - \hat{\mathbf{y}} \\ &= \mathbf{y} - \mathbf{Z}\hat{} \\ &= \mathbf{y} - \mathbf{P}\mathbf{y} \\ &= (\mathbf{I}_n - \mathbf{P})\mathbf{y},\end{aligned}$$

where $\mathbf{I}_n - \mathbf{P}$ is symmetric, idempotent and has trace $(\mathbf{I}_n - \mathbf{P}) = \text{rank}(\mathbf{I}_n - \mathbf{P})\mathbf{y} = n - p$. Note that $\text{rank}(\mathbf{I}_n - \mathbf{P})\mathbf{y} = n - p$ denotes the degrees of freedom of the residuals and is equal to the number of observations, n, minus the number of coefficients (parameters), p.

Theorem 22.2.1.
The vector of fitted values is orthogonal to the vector of residuals, that is

$$\hat{\mathbf{y}}^T\hat{} = \tilde{}^T\hat{\mathbf{y}} = 0.$$

Details of the proof can be omitted.

Proof of Theorem 22.2.1.

$$\begin{aligned}\hat{\mathbf{y}}^T\hat{} &= (\mathbf{P}\mathbf{y})^T(\mathbf{I}_n - \mathbf{P})\mathbf{y} \\ &= \mathbf{y}^T\mathbf{P}^T(\mathbf{I}_n - \mathbf{P})\mathbf{y} \\ &= \mathbf{y}^T\mathbf{P}^T\mathbf{y} - \mathbf{y}^T\mathbf{P}^T\mathbf{P}\mathbf{y} \\ &= \mathbf{y}^T\mathbf{P}\mathbf{y} - \mathbf{y}^T\mathbf{P}\mathbf{P}\mathbf{y} \\ &= \mathbf{y}^T\mathbf{P}\mathbf{y} - \mathbf{y}^T\mathbf{P}\mathbf{y} \\ &= 0,\end{aligned}$$

using that $\mathbf{P}$ is orthogonal ($\mathbf{P}^T = \mathbf{P}$) and idempotent ($\mathbf{P}^2 = \mathbf{P}$).

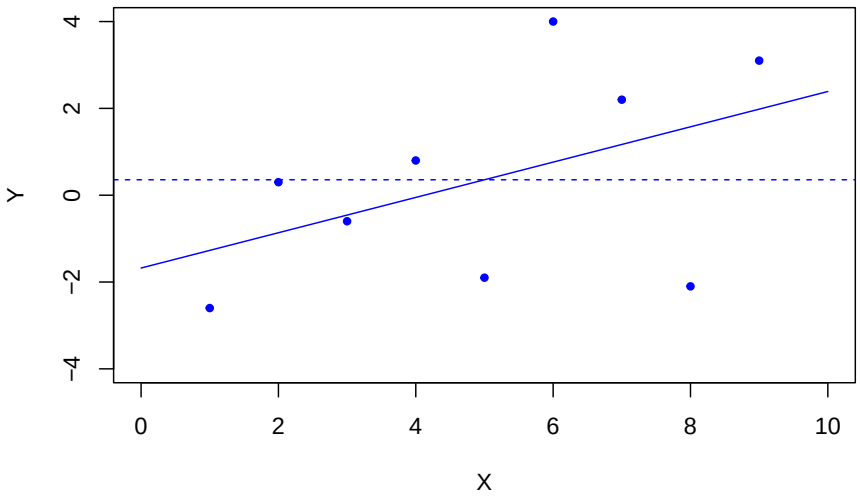
Therefore, $\mathbf{y}$ can be written as a linear combination of orthogonal vectors:

$$\mathbf{y} = \hat{\mathbf{y}} + \hat{}.$$

The normal linear model assumes $\sim N(\mathbf{0}, \sigma^2\mathbf{I}_n)$. We would expect the sample residuals, $\hat{}$ to exhibit many of the properties of the error terms. The properties of $\hat{}$ can be explored via graphical methods as in Section 16.6 and Lab 9: Linear Models.

22.3 Sums of squares

Let y_i be the i^{th} observation, $\hat{y}_i$ be the i^{th} fitted value and $\bar{y}$ be the mean of the observed values.



Lemma 22.3.1. **Model Deviance**

The model deviance is given by

$$D = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2.$$

We have

$$
\begin{aligned}
& & (y_i - \bar{y}) &= (y_i - \hat{y}_i) + (\hat{y}_i - \bar{y}), \\
\implies & & (y_i - \bar{y})^2 &= \left[(y_i - \hat{y}_i) + (\hat{y}_i - \bar{y})\right]^2 \\
& & &= (y_i - \hat{y}_i)^2 + (\hat{y}_i - \bar{y})^2 + 2(y_i - \hat{y}_i)(\hat{y}_i - \bar{y}), \\
\implies & & \sum_{i=1}^{n}(y_i - \bar{y})^2 &= \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2 + 2\sum_{i=1}^{n}(y_i - \hat{y}_i)(\hat{y}_i - \bar{y}).
\end{aligned}
$$

Now,

$$
\begin{aligned}
\sum_{i=1}^{n}(y_i - \hat{y}_i)(\hat{y}_i - \bar{y}) &= \sum_{i=1}^{n}(y_i - \hat{y}_i)\hat{y}_i - \sum_{i=1}^{n}(y_i - \hat{y}_i)\bar{y} \\
&= \sum_{i=1}^{n}\hat{\epsilon}_i\hat{y}_i - \bar{y}\sum_{i=1}^{n}\hat{\epsilon}_i \\
&= \hat{\epsilon}^T\hat{\mathbf{y}} - \bar{y}\sum_{i=1}^{n}\hat{\epsilon}_i \\
&= 0 - 0 \\
&= 0,
\end{aligned}
$$

using that $\hat{\epsilon}$ and $\hat{\mathbf{y}}$ are orthogonal, and that $\sum_{i=1}^{n}\hat{\epsilon}_i = 0$ is one of the normal equations. Therefore,

$$
\sum_{i=1}^{n}(y_i - \bar{y})^2 = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2 .
$$

Definition 22.3.2. **Total sum of squares**

Define SStot $= \sum_{i=1}^{n}(y_i - \bar{y})^2$ as the **total sum of squares**. This is proportional to the total variability in y since SStot $= (n-1)\text{Var}(y)$. It does not depend on the choice of predictor variables in $\mathbf{Z}$.

Definition 22.3.3. **Residual sum of squares**

Define $\text{SSres} = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$ as the **residual sum of squares**. This is a measure of the amount of variability in y the model was unable to explain. This is equivalent to the deviance of the model, that is $\text{SSres} = D$.

Definition 22.3.4. **Regression sum of squares**

Define $\text{SSreg} = \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2$ as the **regression sum of squares**. This is the difference between SStot and SSres and is a measure of the amount of variability in y the model was able to explain.

From our above derivations, note

$$\sum_{i=1}^{n}(y_i - \bar{y})^2 = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2$$
$$\text{SStot} = \text{SSres} + \text{SSreg}$$

Definition 22.3.5. **Coefficient of determination**

The *coefficient of determination* is

$$R^2 = \frac{\text{SSreg}}{\text{SStot}}.$$

The coefficient of determination measures the proportion of variability explained by the regression. Additionally note that:

- $0 \leq R^2 \leq 1$;
- $R^2 = 1 - \frac{\text{SSres}}{\text{SStot}}$;
- R^2 is often used as a measure of how well the regression model fits the data: the larger R^2 is, the better the fit. One needs to be careful in interpreting what "large" is on a case-by-case basis.

Definition 22.3.6. **Adjusted R^2**

The *adjusted* R^2 is

$$R^2_{\text{adj}} = 1 - \frac{\text{SSres}/(n-p)}{\text{SStot}/(n-1)}.$$

The adjusted R^2 is often used to compare the fit of models with different numbers of parameters.

Under the null hypothesis model, $Y_i = \beta_0 + \epsilon_i$ and $\bar{y} = \hat{y}_i$. In this special case,

$$\begin{aligned} \text{SStot} = \text{SSres} &= D, \\ \text{SSreg} &= 0, \\ R^2 = R^2_{\text{adj}} &= 0. \end{aligned}$$

22.4 Analysis of Variance (ANOVA)

Recall from Section 21.4 that the F statistic used in the test for the existence of regression is

$$F = \frac{(D_0 - D_1)/(p-1)}{D_1/(n-p)},$$

where D_1 and D_0 are the model deviances or SSres under the alternative and null hypotheses respectively. We noted above that D_0, the deviance under the null hypothesis is equivalent to SStot under any model.

Definition 22.4.1. **Mean square regression**

The **mean square regression** is the numerator in the F statistic,

$$\text{MSreg} = \frac{D_0 - D_1}{p-1} = \frac{\text{SStot} - \text{SSres}}{p-1} = \frac{\text{SSreg}}{p-1}.$$

Definition 22.4.2. **Mean square residual**

The **mean square residual** is the denominator in the F statistic,

$$\text{MSres} = \frac{D_1}{n-p} = \frac{\text{SSres}}{n-p}.$$

Note the mean square residual is an unbiased estimator of σ^2. Similarly, the **residual standard error**, $\text{RSE} = \sqrt{\text{MSres}}$ is an unbiased estimate of σ.

The quantities involved in the calculation of the F statistic are usually displayed in an ANOVA table:

Source	Degrees of Freedom	Sum of Squares	Mean Square	F Statistic
Regression	$p-1$	SSreg	$\text{MSreg} = \frac{\text{SSreg}}{p-1}$	$F = \frac{\text{MSreg}}{\text{MSres}}$
Residual	$n-p$	SSres	$\text{MSres} = \frac{\text{SSres}}{n-p}$	
Total	$n-1$	SStot		

Definition 22.4.3. **Fuel consumption (continued)** For the data in Section 21.2, Example 21.2.1 (Fuel Consumption) the model

$$\text{fuel} = \beta_0 + \beta_1 \text{dlic} + \beta_2 \text{tax} + \beta_3 \text{inc} + \beta_4 \text{road}$$

was fitted to the $n = 51$ observations with residual standard error, RSE = 64.8912. Summary statistics show Var(fuel) = 7913.88. Complete an ANOVA table and compute R^2 for the fitted model.

We have

- Note $p-1 = 4$, $n-p = 46$ and $n-1 = 50$;
- $\text{SStot} = (n-1)\text{Var(fuel)} = 50 \times 7913.88 = 395694$;
- $\text{MSres} = \text{RSE}^2 = 64.8912^2 = 4210.87$;
- $\text{SSres} = (n-p)\text{MSres} = 46 \times 4210.87 = 193700$;
- $\text{SSreg} = \text{SStot} - \text{SSres} = 395694 - 193700 = 201994$;
- $\text{MSreg} = \text{SSreg}/(p-1) = 201994/4 = 50498.50$;
- $F = \text{MSreg}/\text{MSres} = 50498.5/4210.87 = 11.99$.

Hence the completed ANOVA table is

Source	Degrees of Freedom	Sum of Squares	Mean Square	F statistic
Regression	4	201994	50498.50	11.99
Residual	46	193700	4210.87	
Total	50	395694		

We compare the computed F-statistic, 11.99, with a $F_{p-1,n-p} = F_{4,46}$ distribution to obtain a p-value of $9.331 \times 10^{-7} = P(F_{4,46} > 11.99)$. That is, if the

null hypothesis (no regression parameters $\beta_1 = ... = \beta_4 = 0$) were true, there is probability 9.331×10^{-7} (just under one in a million) of observing an F-statistic larger than 11.99.

Finally, $R^2 = \frac{\text{SSreg}}{\text{SStot}} = \frac{201994}{395694} = 0.5105$.

22.5 Comparing models

Consider two models, M_1 and M_2, where M_2 is a simplification of M_1. For example,

$$\begin{aligned} M_1: &\quad Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_4 X_4 + \epsilon, \\ M_2: &\quad Y = \beta_0 + \beta_2 X_2 + \beta_4 X_4 + \epsilon. \end{aligned}$$

The residual sum of squares from model M_1 will always be less then M_2, but we can test the hypotheses:

$$H_0 : \beta_1 = \beta_3 = 0 \quad \text{vs.} \quad H_1 : \beta_1 \neq 0 \text{ or } \beta_3 \neq 0$$

at significance level α to test if removing these terms significantly increases the residual sum of squares.

Let $D_1 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$ be the model deviance, or SSres, for model M_1.

Let $D_2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$ be the model deviance, or SSres, for model M_2.

The *decision rule* is to reject H_0 if

$$F = \frac{(D_2 - D_1)/q}{D_1/(n-p)} > F_{q,n-p,\alpha},$$

where n is the number of observations, p is the number of parameters in M_1 and q is the number of parameters that are fixed to reduce M_1 to M_2.

For the example above, $p = 5$ and $q = 2$.

Watch Video 32 for a work through of comparing models using the F-distribution. The video uses Example 22.5.1 (Fuel consumption - continued) given below.

Watch Video 32: Model comparison

Example 22.5.1. **Fuel consumption (continued)**
Let Model 1 be

$$\text{fuel} = \beta_0 + \beta_1 \text{dlic} + \beta_2 \text{tax} + \beta_3 \text{inc} + \beta_4 \text{road},$$

and let Model 2 be

$$\text{fuel} = \beta_0 + \beta_1 \text{dlic} + \beta_3 \text{inc}.$$

The residual sum of squares is 193700 for Model 1 and 249264 for Model 2. Test which model fits the data better.

The question is equivalent to testing the hypotheses:

$$H_0 : \beta_2 = \beta_4 = 0 \quad \text{vs.} \quad H_1 : \beta_2 \neq 0 \text{ or } \beta_4 \neq 0,$$

at $\alpha = 0.05$. The decision rule is to reject H_0 if

$$F = \frac{(D_2 - D_1)/q}{D_1/(n-p)} > F_{q,n-p,\alpha} = F_{2,46,0.05} = 3.20.$$

Substituting in the data gives,

$$F = \frac{(249264 - 193700)/2}{193700/(51-5)} = 6.598.$$

Consequently, we will reject H_0. Model 1 fits the data better at $\alpha = 0.05$.

We note that the p-value is $0.0048 = P(F_{2,46} > 6.598)$, which gives very strong support in favour of Model 1.

Let's consider the more general case where the basic model M_1 is

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_{p-1} X_{p-1} + \epsilon.$$

Denote

$$\text{SSreg}(M_1) = \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2 = R(\beta_1, \beta_2, \ldots, \beta_{p-1} | \beta_0),$$

assuming there is a constant in the model.

Our goal is to build a regression model which *best* describes the response variable. Hence we would like to explain as much of the variance in Y as possible, yet keep the model as simple as possible. This is known as the **Principle of Parsimony**. Consequently we want to determine which explanatory variables are worthwhile to include in the final model.

The idea is that explanatory variables should be included in the model if the extra portion of the regression sum of squares, called the extra sum of squares,

which arises from their inclusion in the model is relatively large compared to the unexplained variance in the model, residual sum of squares.

Consider a second model M_2 which is a simplification of M_1, specifically

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_{k-1} X_{k-1} + \epsilon,$$

where $k < p$. Then

$$\text{SSreg}(M_2) = R(\beta_1, \beta_2, \ldots, \beta_{k-1} | \beta_0).$$

Definition 22.5.2. **Extra sum of squares**
The *extra sum of squares* due to the inclusion of the terms $\beta_k X_k + \cdots + \beta_{p-1} X_{p-1}$ in the model is

$$\text{SSreg}(M_1) - \text{SSreg}(M_2).$$

It is denoted

$$R(\beta_k, \ldots, \beta_{p-1} | \beta_0, \beta_1, \ldots, \beta_{k-1}) = R(\beta_1, \beta_2, \ldots, \beta_{p-1} | \beta_0) - R(\beta_1, \beta_2, \ldots, \beta_{k-1} | \beta_0).$$

The extra sum of squares has $q = p - k$ degrees of freedom, where q is the number of explanatory variables added to the reduced model to make the full model.

We can test the hypotheses:

- H_0 : The reduced model, M_2, best describes the data;
- H_1 : The full model, M_1, best describes the data.

The **decision rule** is to reject H_0 if

$$F = \frac{R(\beta_k, \ldots, \beta_{p-1} | \beta_0, \ldots, \beta_{k-1})/q}{\text{SSres}(M_1)/(n-p)} > F_{q,n-p,\alpha}.$$

Rejecting H_0 implies the full model describes the data better, so we should include the variables $X_k, \ldots, X_{p-1}$ in our model.

The test for the existence of regression is a special case of this type of test, where

$$H_0 : \beta_1 = \beta_2 = \cdots = \beta_p = 0,$$

that is, the reduced model is $Y = \beta_0 + \epsilon$. Note that $\text{SSreg}(M_1) = R(\beta_1, \beta_2, \ldots, \beta_{p-1}|\beta_0)$ is the extra sum of squares in this case.

22.6 Sequential sum of squares

Definition 22.6.1. **Sequential sum of squares**
The *sequential sum of squares* for each j, denoted SSseq_i, is

$$R(\beta_j|\beta_0, \beta_1, \ldots, \beta_{j-1}) = R(\beta_1, \beta_2, \ldots, \beta_j|\beta_0) - R(\beta_1, \beta_2, \ldots, \beta_{j-1}|\beta_0)$$

and is the extra sum of squares that one incurs by adding the explanatory variable X_j to the model given that $X_1, \ldots, X_{j-1}$ are already present.

The sequential sum of squares is often given in addition to the basic ANOVA table.

Source	Degrees of Freedom	Sequential Sum of Squares	Mean Square	F statistic
X_1	df_1	SSseq_1	$\text{MSseq}_1 = \frac{\text{SSseq}_1}{\text{df}_1}$	$F = \frac{\text{MSseq}_1}{\text{MSres}}$
X_2	df_2	SSseq_2	$\text{MSseq}_2 = \frac{\text{SSseq}_2}{\text{df}_2}$	$F = \frac{\text{MSseq}_2}{\text{MSres}}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
X_{p-1}	df_{p-1}	SSseq_{p-1}	$\text{MSseq}_{p-1} = \frac{\text{SSseq}_{p-1}}{\text{df}_{p-1}}$	$F = \frac{\text{MSseq}_{p-1}}{\text{MSres}}$
Residuals	$n-p$	SSres	$\text{MSres} = \frac{\text{SSres}}{n-p}$	

Note that given the sequential sum of squares, one can calculate

$$R(\beta_j, \beta_{j+1}, \ldots, \beta_k|\beta_0, \beta_1, \ldots, \beta_{j-1}) = \sum_{i=j}^{k} \text{SSseq}_i.$$

However, one cannot calculate the nonsequential sums of squares in this manner, such as

$$R(\beta_1, \beta_3, \beta_5 | \beta_0, \beta_2, \beta_4).$$

Note that in the fuel example

$$\text{SSreg} = R(\beta_1|\beta_0) + R(\beta_2|\beta_0, \beta_1) + R(\beta_3|\beta_0, \beta_1, \beta_2) + R(\beta_4|\beta_0, \beta_1, \beta_2, \beta_3).$$

Definition 22.6.2. **Partial sum of squares**
The *partial sum of squares* for each j is

$$\begin{aligned} &R(\beta_j|\beta_0, \beta_1, \dots, \beta_{j-1}, \beta_{j+1}, \dots, \beta_{p-1}) \\ &\qquad = R(\beta_1, \beta_2, \dots, \beta_{p-1}|\beta_0) - R(\beta_1, \dots, \beta_{j-1}, \beta_{j+1}, \dots, \beta_{p-1}|\beta_0) \end{aligned}$$

and is the extra sum of squares that one incurs by adding the explanatory variable X_j to the model given that $X_1, \dots, X_{j-1}, X_{j+1}, \dots, X_{p-1}$ are already present.

Note that the F test for testing the hypotheses:

$$H_0 : \beta_j = 0 \quad \text{vs.} \quad H_1 : \beta_j \neq 0$$

at level α, is equivalent to the t test for the individual parameter since $t^2_{n-p} = F_{1,n-p}$.

Example 22.6.3. **Fuel consumption (continued)** For the data in Section 21.2, Example 21.2.1 (Fuel Consumption), we have the following ANOVA output table:

Source	Degrees of Freedom	Sequential Sum of Square	Mean Square
dlic	1	86854	86854
tax	1	19159	19159
inc	1	61408	61408
road	1	34573	34573
Residuals	46	193700	4211

We want to test the following hypotheses:

- H_0 : $Y = \beta_0 + \beta_1 \text{dlic} + \beta_2 \text{tax} + \epsilon$;
- H_1 : $Y = \beta_0 + \beta_1 \text{dlic} + \beta_2 \text{tax} + \beta_3 \text{inc} + \beta_4 \text{road} + \epsilon$.

The decision rule is to reject H_0 if

$$F = \frac{R(\beta_3, \beta_4|\beta_0, \beta_1, \beta_2)/2}{\text{SSres}/(n-p)} > F_{2,n-p,0.05}$$

where

$$\begin{aligned} R(\beta_3, \beta_4|\beta_0, \beta_1, \beta_2) &= R(\beta_3|\beta_0, \beta_1, \beta_2) + R(\beta_4|\beta_0, \beta_1, \beta_2, \beta_3) \\ &= 61408 + 34573 \\ &= 95981. \end{aligned}$$

Hence,

$$F = \frac{95981/2}{4211} = 11.40 > F_{2,46,0.05} = 3.20.$$

Therefore we will reject H_0 at $\alpha = 0.05$. Including the variables *inc* and *road* significantly improves the model. The p-value is $P(F_{2,46} > 11.40) = 9.53 \times 10^{-5}$.

To compare the linear models:

- $H_0: \quad Y = \beta_0 + \beta_1 \text{dlic} + \beta_3 \text{inc} + \beta_4 \text{road} + \epsilon;$
- $H_1: \quad Y = \beta_0 + \beta_1 \text{dlic} + \beta_2 \text{tax} + \beta_3 \text{inc} + \beta_4 \text{road} + \epsilon$

is equivalent to the hypotheses: $H_0 : \beta_2 = 0$ vs. $H_1 : \beta_2 \neq 0$.

The residual sum-of-squares under H_0 and H_1 are 211964 and 193700, respectively. Since the residual degrees of freedom under the full model is 46 the F-statistic is:

$$F = \frac{211964 - 193700}{193700/46} = 4.34.$$

The p-value is $\text{P}(F_{1,46} > 4.34) = 0.0429$ which coincides with the p-value for testing $\beta_2 = 0$ in Section 21.2, Example 21.2.1 (Fuel Consumption).

Task: Session 12

Attempt the **R Markdown** file for Session 12:
Session 12: Linear Models II

Student Exercises

Attempt the exercises below.

Exercise 22.1.
The following R output is from the analysis of 43 years of weather records in California. 10 values denoted {i?} for $i = 1, \ldots, 10$ have been removed. What are the 10 missing values?

```
Call:
lm(formula = BSAAM ~ APMAM + OPRC)

Residuals:
     Min       1Q   Median       3Q      Max
-21893.1  -6742.5   -654.1   6725.7  27061.8

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  16703.9     5033.7   3.318  0.00194 **
APMAM          815.0      501.6   1.625  0.11206
OPRC          4589.7      309.0    {1?}     {3?} {4?}
---
Signif. codes:   0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 9948 on {2?} degrees of freedom
Multiple R-squared: {7?},     Adjusted R-squared: 0.848
F-statistic: {8?} on {9?} and {10?} DF,  p-value: < 2.2e-16

Analysis of Variance Table

Response: BSAAM

          Df     Sum Sq    Mean Sq F value    Pr(>F)
APMAM      1 1.5567e+09 1.5567e+09  15.730 0.0002945 ***
OPRC       1 2.1836e+10 2.1836e+10    {6?} < 2.2e-16 ***
Residuals 40 3.9586e+09       {5?}
---
Signif. codes: 0   *** 0.001 ** 0.01 * 0.05 . 0.1 1
```

Exercise 22.2.
An experiment was conducted to find out how long is a piece of string. Six pieces of string were measured along with their colour.

Length	Colour
9	Orange
28	Grey
8	Pink
31	Grey
6	Pink
11	Orange

a. Write down an appropriate model to test for an association between colour and the length of string. Hence write down the design matrix.

b. Find the least squares estimates for the parameters in your model. You may find the following inverse helpful:

$$\begin{pmatrix} 6 & 2 & 2 \\ 2 & 2 & 0 \\ 2 & 0 & 2 \end{pmatrix}^{-1} = \frac{1}{2} \begin{pmatrix} 1 & -1 & -1 \\ -1 & 2 & 1 \\ -1 & 1 & 2 \end{pmatrix}.$$

c. Find the fitted values and residuals for your model.

d. Calculate the ANOVA table and then use it to test the hypothesis that colour affects the length of string.

Chapter 23

Introduction to R

23.1 What are R, RStudio and R Markdown?

R is a free and widely used statistical language/package. There is a huge range of statistical commands in **R**, from basic summary statistics to cutting edge research applications. It is also a programming environment, so you can soon build up your own routines.

RStudio is a free graphical user interface that makes using **R** more user-friendly.

Almost all practical statistical analysis is carried out on a computer, and so becoming familiar with computer packages and languages is an essential task for any user of statistics.

To help you create beautiful output (HTML pages with mathematics included) we shall use a package called **knitr** which is embedded within some more general **R Markdown** packages, it turns your comments and code into a pretty HTML file. For each computing session I will give you an "R Markdown" file in RStudio (it ends in .Rmd) and then you can use knitr in RStudio to create the HTML. Note that you will need to edit the R Markdown file to answer the questions it contains.

23.2 Starting RStudio on the UoN Network

First of all log into the computer system. You can then start **RStudio** by going to the start menu and selecting

Start → UoN Applications → (UoN) RStudio (x.x.x)

where (x.x.x) is the latest version of **RStudio** available.

R is a command line based language, so you will need to type in the commands with any options and arguments. When **RStudio** starts a console window is opened. It is here that you type in the commands.

23.3 Downloading R and RStudio

It is recommended that you download **RStudio** onto your own computer to have **R** available when both working online and offline.

To run **RStudio** on your own computer then you first need to download **R** from CRAN (Comprehensive R Archive Network):
Download R
and then you can download **RStudio** from
Download R Studio

Note that both **R** and **RStudio** are free.

You can also find additional documentation on **R**, including introductory material, at the CRAN site.

23.4 Getting started in R

Once you have either accessed **R** through the UoN Network or downloaded and opened **RStudio**, watch the following Video: Introduction to R which gives an introduction to **R** and the basics of **RStudio**. It might be helpful, if possible, to simultaneously have **RStudio** open and watch the video so that you can get a feel for using **RStudio**.

Watch Video R1: Introduction to R

The **R** script file featured in Video: Introduction to R can be downloaded at:
Session 0: Introduction to R script
This file is highly recommended if you don't have any previous **R** experience.

Chapter 24

What is R Markdown?

In this Section, we give a brief introduction to **R Markdown**. We present a brief summary of the key features, R code, text and maths, which make up an **R Markdown** file. Finally, there is a video which works through the construction of a simple R Markdown file.

24.1 Getting started

Embarking upon writing an **R Markdown** file is rather daunting at first. **R** provides a *simple* **R Markdown** template which launches when you create a new **R Markdown** file. Whilst this is helpful, it is not easy going for somebody who is new to **R**. Therefore we will start with pre-prepared **R Markdown** templates for you to work from and as the Programme progresses you will develop your skills and begin to be able to construct your **R Markdown** files from scratch.

This document is designed to help navigate you around **R Markdown** documents and to *knit* (compile) a html file with your output. We will focus on inputting **R** code (including) and text into an **R Markdown** template. The end of this document touches upon the inclusion of mathematics.

Figure 24.1 show the start of an R markdown file.

The file header is:

```
---
title: "My R Markdown"
output: html_document
---
```

All R Markdown will have a header of this form, specifying the title and output type. The title is self-explanatory and you can change to whatever you choose.

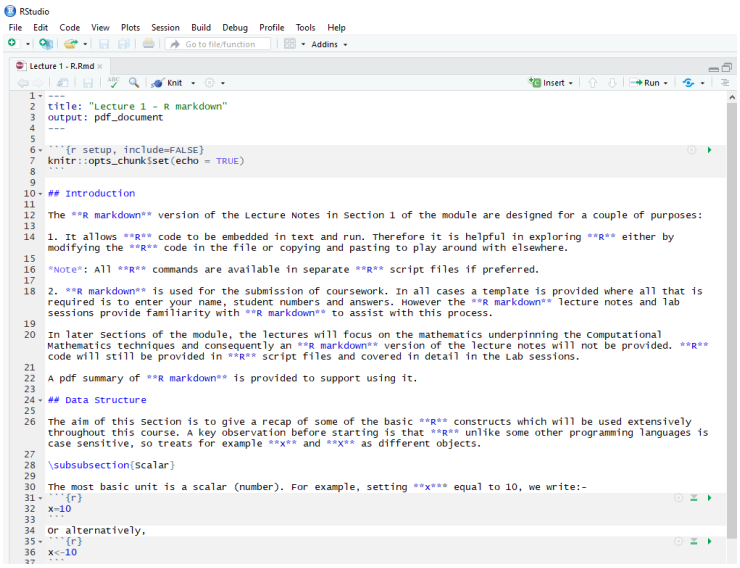


Figure 24.1: Start of an R markdown file.

The output states what sort of document is produced when markdown is run. The two main options are **html_document** and **pdf_document** which produce a html file and a pdf file as output, respectively.

In order to construct the html or pdf file output you need to compile the file using the **Knit** icon in the menu bar at the top of the script window which is circled in Figure 24.2 show the start of an R markdown file.

24.2 R in R Markdown

Immediately below the title we have:

This sets up the **R** code. The **include=FALSE** means that information from the setup is not included in the output file. The **echo=TRUE** means that the default option when running **R** code is to produce both the **R** code and the resulting output in the html/pdf file. For the purposes of assessment, you will often set **echo=TRUE** so that the code can be seen. However, if you are producing a document for other purposes you will often not want the **R** code to be shown. For any section of **R** code you can locally override the global decision (include or exclude **R** code).

Once you're working with an **R Markdown** document you can insert chunks of **R** code by clicking on Insert and **R**. (You will notice other options such as Python are available.) The syntax is as follows. Note that the apostrophes are backwards, the key on the keyboard is normally found top left (next to 1). It's

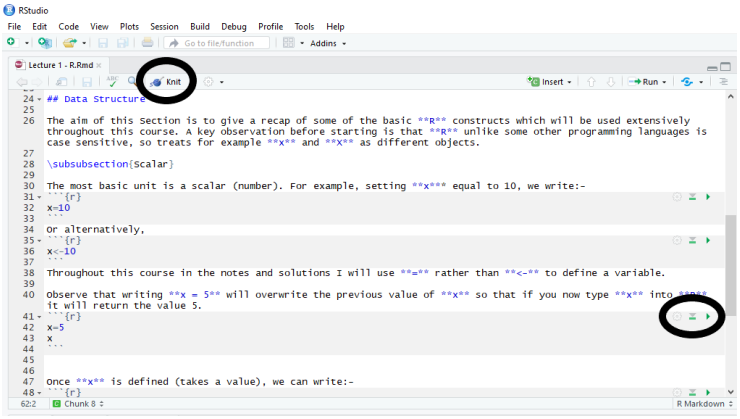


Figure 24.2: R markdown image highlighting Knit button and R segment run options.

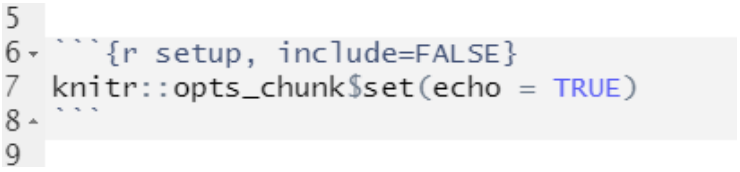


Figure 24.3: **R** Setup code.

often called backquote, or backtick, or grave accent.

```
```r
# Insert your lines of R code
# in between these triple backquotes.
# Each such construction is called an R code chunk.
```
```

Remember that hashtag, #, signifies to **R** that all the rest of the text on that line is a comment and not **R** code. Therefore the above *code* will do nothing.

If you want to run **R** code to test it without using the Knit button to construct the output file, you can use the buttons on the right hand side of the **R** code segments. These buttons are circled in Figure 24.2. The green triangle pointing right runs that segment of code, whilst the grey triangle pointing down with a green bar underneath runs all the **R** code in the document up to this point. Figure 24.4 illustrates using the green button on a short **R** code segment:

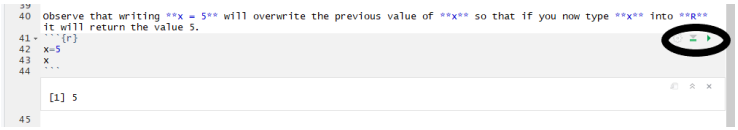


Figure 24.4: Running a segment of **R** code within R markdown, see lines 40-45.

Running segments of **R** code is very useful as the **R markdown** file will not **knit** if there are any errors in the code. An example is given in Figure 24.5 where the line 216 asks **R** to sum two matrices which are different sizes. **R markdown** gives an error message which notifies us that the error is linked to **R** code segment starting at line 215.

If you find an error in your code the first thing to do is to try and fix it. *i.e.* Code debugging. However, sometimes you just won't be able to see what the problem is. In such cases you can include your attempt at the **R** code and tell **R markdown** not to run the **R** code (to create an error message). This can be done by setting `eval=FALSE`.

Using this option allows you to present code and comment that it's not quite working.

```
```r
s <- (-3)^^^0.5 # I'm not sure why, but this doesn't work.
```
```

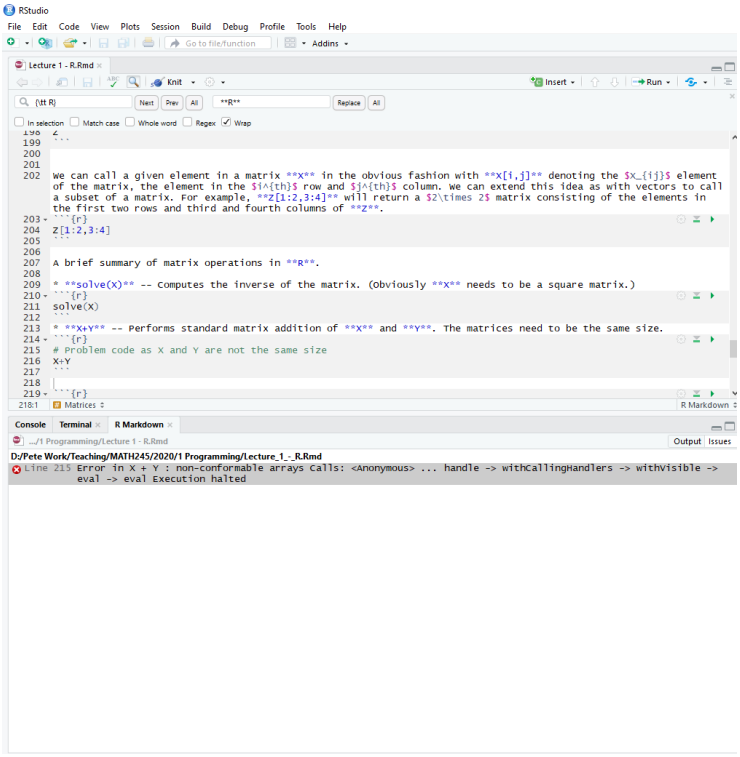


Figure 24.5: Error message when **knitting** R markdown. Error linked to **R** code segment starting at line 215.

Another option available is `results = 'hide'`. Hiding results causes the output HTML not to include the results that **R** calculates and displays on the screen (but it does still run the code, in contrast to eval above).

````
```r
# This boring part creates a vector in a tedious way.
A <- rep(1,2)
A
A <- cbind(A,5)
A
A <- rbind(A,A)
A
cat (A)
```
````

24.3 Text in R markdown

Text output can just be written as usual, outside of these **R** chunks. **R** variables can be used outside of chunks if you wish, using a `r yourmaths` command (use a single backquote at each end, follow the first backquote by an r and a space to the **R** code you want to implement). Those of you with knowledge of LaTeX could use $ and $$ commands if you like, to get nicely formatted mathematical equations but this isn't essential. **R Markdown** allows for many shortcuts for formatting headings, bullet points and the like. For example, to produce **bold** and *italic* text we use `**bold**` and `*italic*`. Headings of various levels are given by #, for example, `# Heading 1`, `## Heading 2`, ... The fewer # the higher the level of Heading (the larger) the text.

Read the **R Markdown** cheat sheet in **RStudio** for help, see:

https://www.rstudio.com/wp-content/uploads/2015/02/rmarkdown-cheatsheet.pdf

24.4 Mathematics in R Markdown

For completeness, we include a short summary of including mathematics in **R Markdown**. This can be skipped for now.

Mathematical expressions are placed between a pair of $ signs (maths mode), or the case of an equation is place within `\[  \]`. Note that \ is used to initiate many commands in LaTeX.

The key operations are:

1. **Superscript** To insert a superscript we use `^`. For example, to write x^2,

we write `$x^2$`. If we want to include a superscript involving more than one expression, we place the expression to form the superscript in {}. For example, e^{x+2} is given by `$e^{x+2}$`.

2. **Subscript** To insert a subscript we use `_`. For example, to write y_i, we write `$y_i$`. The same rule concerning placing longer expressions in {} applies for subscripts. If we want to combine sub- and superscripts we can put either the sub- or superscript first. For example, both `$x_j^3$` and `$x^3_j$` produce x^3_j.

3. **Greek Letters** These can also be written in maths mode and we insert to produce the desired letter. For example, `$\beta$` gives β.

4. **Fractions** To produce a fraction we can use `$\frac{A}{B}$`, which will give $\frac{A}{B}$. We can replace A and B by whatever mathematical expression we want with A and B denoting the numerator and denominator, respectively.

5. **Mathematical symbols** For an almost complete catalogue of mathematical symbols, see for example,

https://oeis.org/wiki/List_of_LaTeX_mathematical_symbols

For example, `$\sin (x)$`, `$\leq$`, `$\triangle$` and `$\leftarrow$` produce $\sin(x)$, $\leq$, $\triangle$ and $\leftarrow$, respectively.

We can place more than one expression within the mathematics mode. For example, $x^2 + \alpha = 7$ is generated by `$x^2 + \alpha = 7$`. If we want to put our mathematics expression as an equation on its own line, we use `\[x^2 + \alpha = 7\]` which gives

$$x^2 + \alpha = 7.$$

24.5 Worked Example

We conclude with a video which works through an example of creating a simple R Markdown file.

Watch Video R2: Introduction to R Markdown